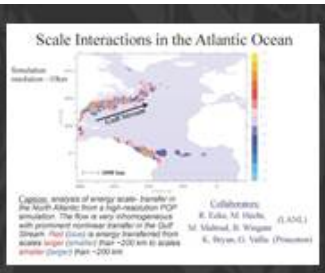

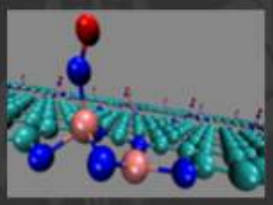

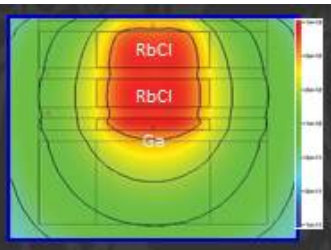

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June 6, 2012

Abstract Book

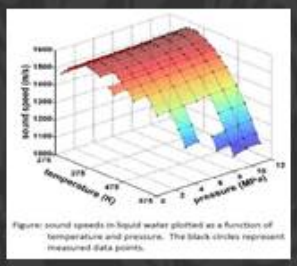


Figure: sound speeds in liquid water plotted as a function of temperature and pressure. The black circles represent measured data points.

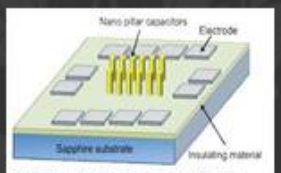


Fig. 1: Schematic image of nanopillar capacitor arrays for single neuron detection. Each nanopillar is connected to each electrode under insulating material. Thus, each nanopillar is perfectly electronically-isolated to each other.

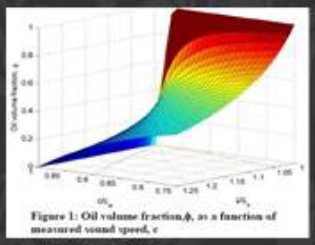
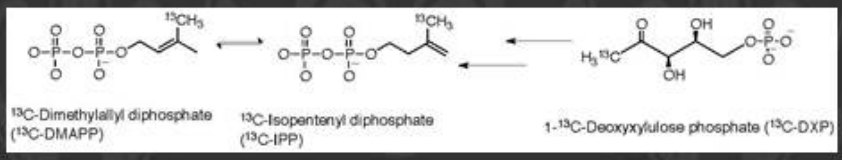
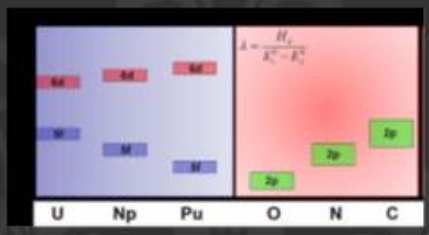
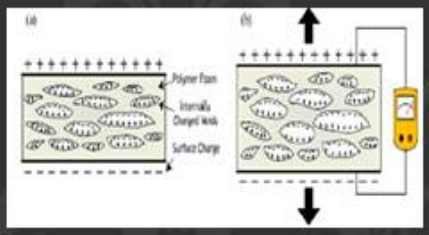
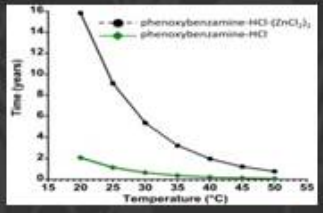


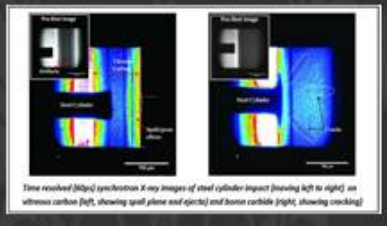
Figure 1: Oil volume fraction,ϕ, as a function of measured sound speed, c



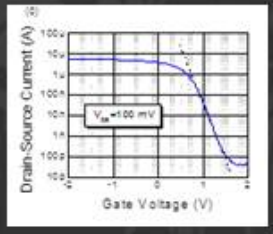








Time resolved (60ps) synchrotron X-ray images of steel cylinder impact (moving left to right) on vitreous carbon (left, showing spall plane and ejecta) and boron carbide (right, showing cracking)



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John Yeager, WX-9

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Accelerator Operations and Technology Division
AOT-ABS

Name	Jeffrey Kolski	LA-UR 11-12226
Groups:	AOT-ABS and AOT-OPS	
Mentors:	Robert Garnett, Rodney McCrady, and Thomas Spickermann	
Field of Study:	Physics	
Discipline:	Accelerator	
Appointment:	Postdoc Research Associate	
Poster Title:	"Diagnostic" Pulse for Single-Particle-Like Beam Position Measurements during Accumulation/Production Mode in the Los Alamos Proton Storage Ring	

ABSTRACT

Beam position monitors are the primary diagnostic in the Proton Storage Ring (PSR) at Los Alamos National Laboratory (LANL). Injecting into a circular accelerator for one turn can be approximated transversely as single-particle injection with initial betatron amplitude and angle, x0 and x0' respectively, also known as the injection offset. The turn-by-turn beam position data of the single-turn injected beam allows measurement of the betatron tune, closed orbit, and injection offset (the x0 and x0' at the injection point). However in accumulation/production mode, multiple turns are injected into the accumulator ring, the transverse phase space is quickly filled, so there is no coherent transverse betatron motion, and only the closed orbit may be measured by the beam position monitors. The important injection offset parameter, which determines the accumulated beam size and is very sensitive to steering upstream of the ring, is not measurable during production. We describe here our approach for measuring the injection offset during accumulation/production mode machine cycles by injecting an additional "diagnostic" beam pulse into the PSR ~50 us after the accumulated beam is extracted. We also study the effects of increasing the length of the rf gate in the linac to accommodate the "diagnostic" pulse on the beam position, transverse size, and loss.

Name	Xiaoying Pang	LA-UR 12-20963
Group:	AOT-ABS	
Mentors:	Lawrence Rybarcyk and Robert Garnett	
Field of Study:	Physics	
Discipline:	Accelerator Physics	
Appointment:	Postdoc Research Associate	
Poster Title:	High Performance Beam Dynamics Simulator for the LANSCE Linear Accelerator	

ABSTRACT

The Los Alamos Neutron Science Center provides the scientific community with neutron and proton beams for use in a diverse set of fundamental and applied research activities. At the heart of the facility is a half-mile long, room-temperature linear accelerator. It is comprised of thousands of electromagnetic elements, such as magnets and radio-frequency (RF) cavities that focus, steer and accelerate the H+ and H- beams from energies of a few electron volts (eV) up to 800,000,000 eV. At the end of the linear accelerator, the speed of particles can reach about 84% of the speed of light. Due to the complexity of the accelerator systems and the limited number of diagnostic tools with which to measure the beams, very limited information can be obtained about the beam dynamics inside the accelerator. During routine operation of the facility, system set points are frequently adjusted with a goal of maintaining minimal beam loss. However, without detailed knowledge of the beam distribution and the effect of the adjustments on it, these changes can potentially lead to degradation in beam quality and higher losses downstream. A more desirable situation will be one where knowledge of the beam distribution along the linear accelerator is available in a timely fashion so that the effect of any operational parameter change can be assessed, more metrics associated with beam quality, not only the beam spill can be estimated. For these reasons we are pursuing a high performance beam dynamics simulator that when linked to the accelerator control system will track changes to system parameters and in rapid response provide valuable insight into the beam motion and quality. The core of this simulator is based upon the multi-particle beam dynamics FORTRAN code PARMILA, but implemented in C++ using NVIDIA's CUDA technology for Graphics Processing Unit (GPU). The GPU hardware was chosen for its inexpensiveness, general availability and great parallel computing performance. Beam dynamics algorithms are recast to maximize the benefit of GPU architectures and a substantial speedup was obtained. So far, the simulator has demonstrated its capabilities of soliciting real-time operational parameters through the accelerator control system, quickly updating the simulation and displaying user-requested beam quality metrics at any location along the accelerator. A demonstration on the 100-MeV Drift Tube Linac (DTL) accelerator will be presented. Details regarding the approach, benefits and performance will also be included.

Bioscience Division
B-7

Name	Amber Nagy	LA-UR 12-20952
Group:	B-7	
Mentors:	Rashi Iyer and Bob Williams	
Field of Study:	Bioscience	
Discipline:	Nanotoxicity	
Appointment:	Postdoc Research Associate	
Poster Title:	Development of Next-Generation Toxicological Models for Human Risk Assessment	

ABSTRACT

The field of nanotechnology has exploded in the past decade while conclusive data regarding health consequences from consumer and occupational exposure to nanomaterials has lagged. One source of this information gap is the lack of reliable, reproducible toxicological models from which predictions and recommendations can be made regarding nanomaterial safety. To address this disparity, the focus of our research is to develop accurate, physiologically relevant human toxicological models to understand risks and consequences surrounding nanomaterial exposure. The proposed approach is based on the hypothesis that reconstructed human tissue equivalents can serve as highly relevant bio-assessment platforms for the risk assessment of a multitude of new nanomaterials. Such a platform integrates the reliable, rapid and high-throughput methodology of in vitro cell based assays with the accuracy and relevance of in vivo platforms making them excellent surrogate models. Because inhalation is a primary exposure pathway for particulates, therapeutics and chemicals, this study focused on the development of in vitro human pulmonary models. We developed a 3-D in vitro human lung tissue construct with highly differentiated cells including, ciliated and mucosal cells, that closely represent the functional and anatomical properties of the lung. Prior to using this platform for bioassessment of nanomaterials, we validated this model using well-established lung toxicants, asbestos and silica, with known parameters of lung pathology.

Three key physicochemical properties of semiconductor nanomaterials – composition, shape and charge – were tested in human primary bronchial epithelial cells (NHBEs) versus 3D human in vitro lung tissue. Both monolayer cultures and in vitro lung tissues were exposed to CdSe or InP quantum dots (QDs) to understand the impacts of nanomaterial composition. Cells and in vitro lung tissue were also exposed to QDs or nanowires (NWs) to gain insight into how shape and charge influence pulmonary responses. End-point readouts included analyses of cellular/tissue and molecular level responses, such as reactive oxygen species (ROS), proliferation, necrosis, apoptosis and changes in gene expression.

Significant property-dependent differential responses in both cells and in vitro lung tissues were observed. Composition and charge played a significant role in QD-induced biological responses, followed closely by shape characteristics, where positively charged materials were more toxic than negatively charged QDs. Gene level analysis suggested that perturbations in mitochondrial processes might be the driver for the differential observed toxic effects. Neither of these trends were apparent in exposed tissues; rather, genes associated with tissue invasion were upregulated in response to QD exposure irrespective of QD charge.

Our data suggest that cell monolayer responses might be significantly different from those elicited in tissue cultures; therefore, care must be taken when drawing conclusions from monolayer cell culture experiments. With regards to the impact of physicochemical properties on nanobio interactions, size, shape and composition have all emerged as important factors, with charge playing a pivotal role. Current research is focused on the development of an artificial lung that will accurately mimic the anatomical and structural characteristics of the human lung enabling respiratory gas exchange function.

B-8

Name	Marc-Michael Blum	LA-UR 12-20981
Groups:	B-8 and B-7	
Mentors:	Cliff Unkefer and Robert Williams	
Field of Study:	Bioscience	
Discipline:	Structural Biology, Enzymology	
Appointment:	Director's Postdoc Fellow	
Poster Title:	Datamining High Quality Structural Models - Understanding 6-Fold Beta-Propeller Proteins	

ABSTRACT

More and more protein structures are obtained by experimental techniques such as X-ray crystallography or NMR and the Protein Database (PDB) has now more than 80,000 entries. However this is an insignificant number compared to the number of protein sequences obtained from genomics, Therefore the use of high quality structural models obtained computationally can augment experimental data and lead to new insight in protein structure and function.

Beta-propeller proteins are of high relevance due to their robust fold and high stability. They exist with blade numbers from 4 to 10 but our special interest is in those propeller proteins with six blades. Naturally occuring 6-fold beta-propellers in the N6P superfamily (Nucleophilic attack 6-fold beta-propellers, >2500 sequences) include human Paraoxonase 1 (PON1) and squid diisoproplyl fluorophosphatase (DFPase). Both enzymes are capable of detoxifying organophosphorus nerve agnets such as Sarin or Soman. Other members of the superfamily include strictosidine synthase and several gluconolactonases. A unique characteristic of those N6P members that have been characterized experimentally is a very high degree of structural similarity despite rather low sequence identity (in general 20% and lower).

We have started to obtain high quality structural models of a curated subset of the N6P superfamily using the I-TASSER software that was modified by us and coupled to the Python based structural bioinformatics framework Biskit. Combined with MD simulations using the GROMACS package first results indicate that we will understand the structural underpinnings of the fold to much larger extend than today. Successful completion of this work will enable us to design de-novo beta-propeller proteins with tailored enzymatic activities. This is of high relevance for several pillars of LANL's mission such as bioenergy and threat reduction (chem-bio defense).

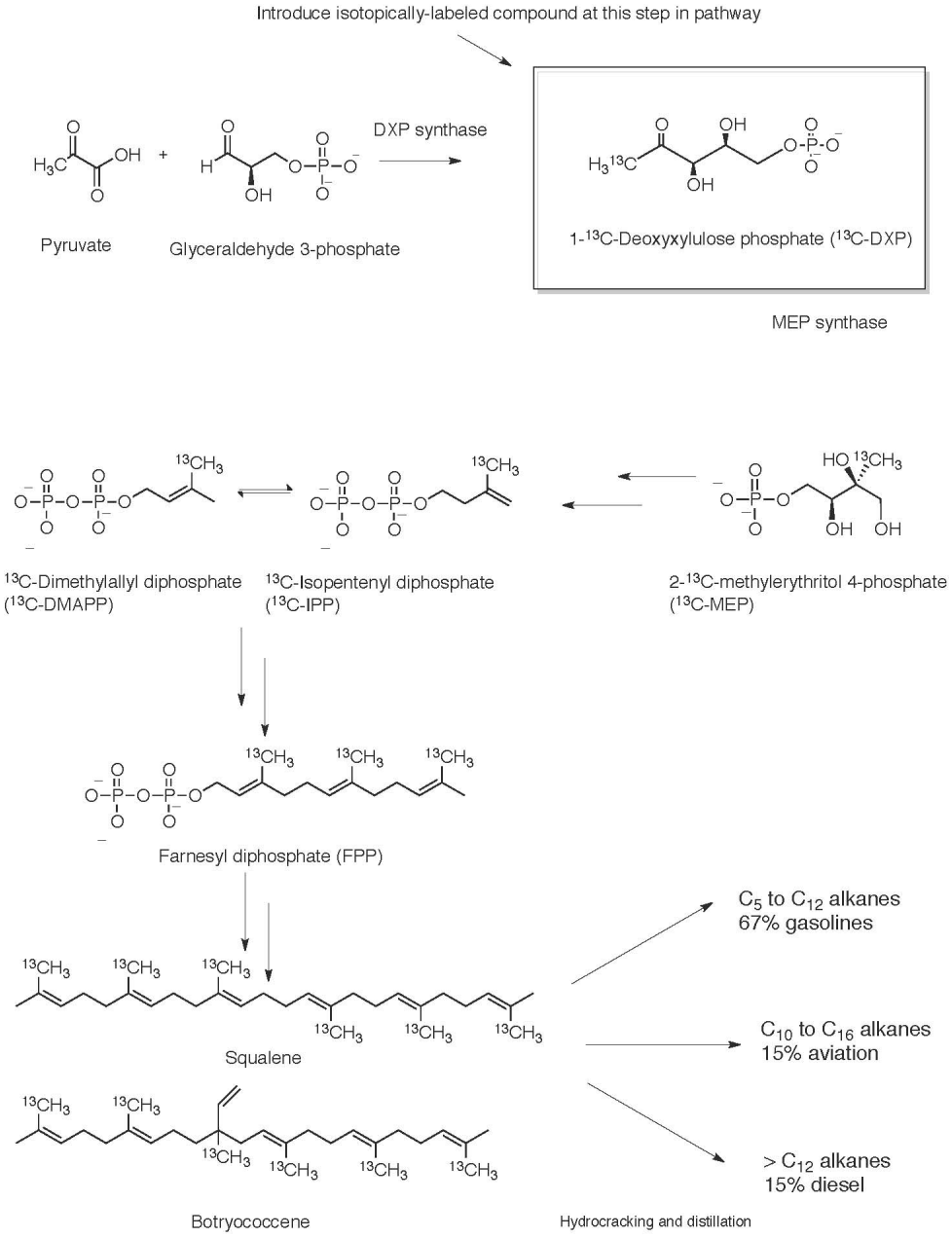
Name	Sarah Sewell	LA-UR 12-20645
Group:	B-8	
Mentor:	David Fox	
Field of Study:	Bioscience	
Discipline:	Bioenergy	
Appointment:	Postdoc Research Associate	
Poster Title:	Monitoring the Distribution of Isoprenoids from the MEP Pathway in Botryococcus Braunii	

ABSTRACT

Molecules known as isoprenoids constitute the largest class of chemical natural products, with over 50,000 identified members. They are present in many pharmaceutical, nutraceutical, and biofuel compounds. All of these products are derived from the chemical compounds isopentenyl diphosphate (IPP), and dimethylallyl diphosphate (DMAPP). IPP and DMAPP are produced via a metabolic route known as the MEP (methylerythritol phosphate) pathway. Improving the production of both IPP and DMAPP would be useful for industrial applications. As such, we have developed a method for tracking the metabolic products through an isotopically-labeled intermediate of the MEP pathway with the ultimate goal of engineering organisms to produce these precursors in higher yield.

The microalga Botrycocccus braunii race B is a prolific isoprenoid-producing organism, however this microbe grows at extremely slow rates thus precluding its use for practical biofuel applications. The enzymes responsible for high isoprenoid production occur exclusively through the MEP pathway. We are pursuing engineering in B. braunii specific MEP pathway genes into algal production strains in order to improve isoprenoid production while maintaining relatively fast growth rates. Our synthetic isotopically-labeled intermediate will provide a convenient handle for tracking improved isoprenoid distribution in the engineered algae through standard analytical techniques.

Name	Sarah Sewell (continued)	LA-UR 12-20645
Group:	B-8	
Mentor:	David Fox	
Field of Study:	Bioscience	
Discipline:	Bioenergy	
Appointment:	Postdoc Research Associate	
Poster Title:	Monitoring the Distribution of Isoprenoids from the MEP Pathway in Botryococcus Braunii	



B-9

Name	Ramesh Jha	LA-UR 12-20784
Groups:	B-9 and B-8	
Mentors:	Charlie Strauss and David Fox	
Field of Study:	Bioscience	
Discipline:	Protein Engineering	
Appointment:	Postdoc Research Associate	
Poster Title:	Computational Prediction of Mutations for Altered Sensitivity and Specificity of a Sensor to Detect Peak Concentration of Lipids in Algae	

ABSTRACT

Lipid extraction from algae needs intensive mechanical and chemical treatments that cause a major barrier to its commercial viability for biofuel production. A biosensor that detects the peak concentration of lipids in algae cells and promote a self-lysis will be an important step towards the cost reduction of downstream processing. We chose a bacterial transcription factor, FadR that can bind to lipids of carbon chain length 12 to 22 and induce the gene attached to the promoter. Computational prediction using Rosetta was carried at different levels to identify the mutations on FadR protein or FadR operator sequence for altered sensitivity or specificity towards lipids. In the first approach, we tried to predict a mutation on the operator for a tighter interaction so that a higher concentration of lipid is required. Apparently, FadR-operator native interaction is already tightest possible protein-DNA interaction (0.2 nM). In a second approach, we mutated the lipid-binding pocket for weakening the interaction between the lipid and FadR, which will result in reduced sensitivity for lipids. In a third approach, we aimed at improving the binding affinity of FadR-operator, by mutating the protein. Finally, we tried to change the specificity of the FadR for longer lipids especially oleate (C18:1).

Compared to the growth stage, lipid content of model green algae (Chlamydomonas reinhardtii) increases 2 to 11 fold in the nitrogen deprived state while oleate shows 5 to 27 fold increase in the relative concentration. Approaches 1-3, aim at reduced sensitivity of FadR for lipids so that a higher concentration of lipids (that correspond to peak lipid production stage) is required for inducing the transcription factor. The final approach is aimed at altering the specificity of FadR for a lipid that undergoes a maximal change in concentration upon reaching a nitrogen deprived state. We plan to use lysin gene downstream of the FadR promoter, which get expressed at the peak of lipid production and that results in an enzyme production involved in degradation of cell wall and ultimately release of lipids in the medium.

Chemistry Division
C-IIAC

Name	Jonathan Engle	LA-UR 12-20658
Group:	C-IIAC	
Mentors:	Francois Nortier and Eva Birnbaum	
Field of Study:	Physics	
Discipline:	Accelerator Production of Radionuclides	
Appointment:	Postdoc Research Associate	
Poster Title:	Preliminary Investigation of Parasitic Radioisotope Production using the LANL IPF Secondary Neutron Fux	

ABSTRACT

Introduction: The Isotope Production Facility (IPF) at Los Alamos National Laboratory produces ^{82}Sr, ^{68}Ge, ^{72}Se, and other isotopes using 100 MeV protons. The IPF's high beam current and lengthy irradiations produce a secondary neutron flux with a utilitarian scale that is beyond the reach of medical cyclotrons and energetically distinct from reactor neutron fluxes. This neutron field will likely broaden the portfolio of radioisotopes sourced from and studied at Los Alamos facilities. Current simultaneous production of ^{82}Sr and ^{68}Ge results in the emission of 10^{17} neutrons in a single run (4π), or ~10^{12} n/s/cm^2, values comparable to fluxes produced in medium intensity research reactors.

Material and methods: The current IPF target stack situates 3 encapsulated target pucks in the path of a 230 μA proton beam, which enters the front face of the first target at approximately 93 MeV. This geometry has been reproduced in Monte Carlo Neutral Particle-eXtended (MCNPX/CINDER90) simulations. Spatial mesh-tally binned neutron fluxes from these simulations have identified locations in the target carrier which maximize exposure to the neutron fluence and are facile to repurpose as carriers of target materials (Fig. 1). MCNPX simulations also describe the energy dependence of the neutron spectrum, which is relatively constant throughout the target geometry. MCNPX was also used to model the ^{184}W(n,α)^{181}Hf reaction during experiemental production of ^{186}Re with a 25 g $^{nat}WO_3$ target for comparison with measured values after chemical separation. To confirm the results of these simulations, a threshold activation experiment will be used to unfold neutron fluence energy distributions from known cross sections and yield measurements of irradiated foils. The SAND-II nuclear code will be used to simplify computation (1). Monoisotopic foil materials with smoothly varying σ(E) for neutron activations and a selection of reaction threshold energies are being prepared for resumption of IPF beam in July 2012: ^{27}Al(n,α)^{24}Na, ^{64}Zn(n,p)^{64}Cu, ^{58}Ni(n,p)^{58}Co, ^{62}Ni(n,α)^{59}Fe, ^{197}Au(n,2n-4n)$^{194-196}$Au, ^{209}Bi(n,2n-5n)$^{205-208}$Bi, and ^{89}Y(n,p)^{89}Sr.

Results: MCNP predicts a total (4π) average flux of 10^{14} n/s/cm^2 around the target carrier (Fig 1). This neutron energy distribution is graphically shown in Fig 2. For the ^{nat}WO3 irradiation, MCNPX/CINDER90 predicted a yield of 0.05 ± 0.02 μCi, in reasonable agreement with HPGE γ-spectroscopy's measured values of 0.02 μCi after separation chemistry.

Conclusions: The neutron flux, once characterized, can be used as a tool for materials science development and for the production of radioisotopes in the service of the larger scientific community. The possibilities include small amounts of ^{67}Cu, ^{225}Rn, ^{103}Pd, ^{142}Pr, ^{125}Sb, ^{153}Sm, and others.

Name	Jonathan Engle (continued)	LA-UR 12-20658
Group:	C-IIAC	
Mentors:	Francois Nortier and Eva Birnbaum	
Field of Study:	Physics	
Discipline:	Accelerator Production of Radionuclides	
Appointment:	Postdoc Research Associate	
Poster Title:	Preliminary Investigation of Parasitic Radioisotope Production using the LANL IPF Secondary Neutron FLUX	

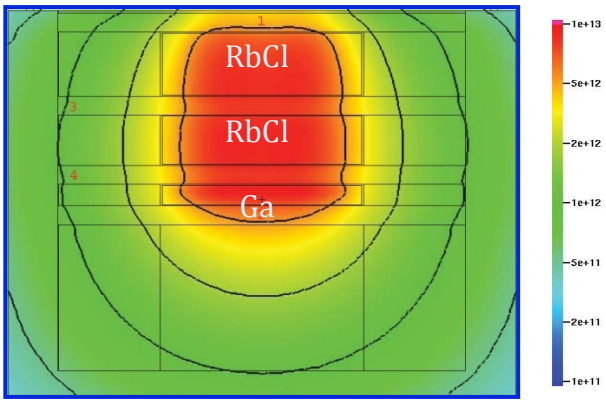


Fig. 1. MCNPX mesh tallies of secondary neutron flux during a 200 μA irradiation (fluxes are in n/s/cm^2 and are independent of energy distribution).

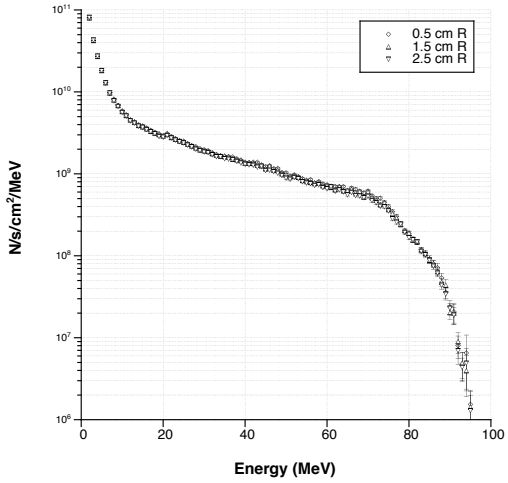


Fig 2. Ring detector tallies for r ≤ 0.5 – 2.5 cm behind Ga target at 200 μA.

References: 1. W N McElroy et al., U.S.A.F. Weapons Laboratory, Technical Report No. AFWL-TR-67-41, 1, 1967.

Acknowledgments, disclosures and funding: We are grateful to the DOE Office of Science for their financial support.

C-NR

Name	Brent Matteson	LA-UR 12-20728
Group:	C-NR	
Mentor:	Warren Oldham	
Field of Study:	Chemistry	
Discipline:	Radiochemistry	
Appointment:	Postdoc Research Associate	
Poster Title:	Radionuclides in Redistributed Sediments and Ash from the Las Conchas Fire in Northern New Mexico	

ABSTRACT

In June of 2011, a tree fell onto a power line on residential property, igniting the 156,000 acre Las Conchas fire within Northern New Mexico's Jemez Mountains. In the weeks following the fire, heavy rainfall caused extensive flooding and erosion of surface sediments and ash from the affected areas. Samples from these mud and ash flows were collected from along a local highway that bisected the burned area and were analyzed for certain anthropogenic and natural radionuclides. These collections were analyzed for 137Cs and Pu, which were originally deposited as global fallout during the era of atmospheric nuclear testing, and were compared to the concentration of natural U and 210Pb isotopes. A striking and consistent correlation was found between elevated levels of Pu and unsupported 210Pb. The latter isotope is continuously deposited onto the surface layers of the forest as a result of radioactive decay of the noble gas, 222Rn. This observation suggests that prior to the fire, both these nuclides had been immobilized into the organic-rich surface of the forest floor. This study provides insight into the mobility, redistribution, and concentration of anthropogenic radionuclides as a result of forest fires. Specifically, measurements of Pu in eroded sediments may ultimately provide a useful tracer of the organic-rich surface material that was lost during the wildfire event.

Name	Gencho Rusev	LA-UR 12-01657
Group:	C-NR	
Mentors:	Todd Bredeweg and Marian Jandel	
Field of Study:	Physics	
Discipline:	Nuclear Physics	
Appointment:	Postdoc Research Associate	
Poster Title:	Gamma-Ray Cascade Transitions in 112Cd and 114Cd Following Capture of Epithermal Neutrons	

ABSTRACT

The nature of gamma-rays emitted from excited nuclei is either deterministic or stochastic. Study of deterministic transitions, such as intra-band transitions in rotational or vibrational bands, leads to valuable information on the structure of the nucleus. On the other hand, stochastic transitions represent the chaotic nature of the nucleus, which is usually difficult to predict. We present research on properties of gamma-ray transitions from excited compound nuclei, Cd-112 and Cd-114, created in neutron capture reactions. Experiments were performed using the Detector for Advanced Neutron Capture Reactions at the Los Alamos Neutron Science Center. Experimental results are compared with Monte Carlo simulations of the gamma-ray transitions in the nucleus. We focused on studying the stochastic transitions in the Cd isotopes because Cadmium is used as a standard shielding material for thermal neutrons and an accurate modeling of gamma-ray emission that follows neutron-capture reaction becomes crucial for building radiation protection systems. In addition, neutron-capture experiments on the Cd isotopes are relevant to nuclear structure since they are classical vibrational nuclei and also to nuclear astrophysics, for example, Cd-110 is a pure s-process nucleus with abundance not affected by any s-process branching paths, therefore it is an important abundance-normalization nucleus in the astrophysical network calculations.

Name	Mindy Zimmer	LA-UR 12-20123
Group:	C-NR	
Mentors:	William Kinman and Rob Steiner	
Field of Study:	Chemistry	
Discipline:	Clean Chemistry/Nuclear Forensics	
Appointment:	Postdoc Research Associate	
Poster Title:	A Novel Method for the Measurement of Trace Elements in Uranium-Rich Materials	

ABSTRACT

A new method for the measurement of trace elements in uranium ore concentrates (UOC) was developed. The trace element composition of a UOC, particularly the abundance of rare earth elements (REE), provides a useful tool for analysis of material source and process history. A number of UOC trace element methods have been described in the literature. The analytical approach described here, however, differs in the choice of dilution and analysis scheme, use of interference correction, internal standard choice for drift correction, and the rinsing and calibration methodologies employed. Trace element concentrations are determined using two sets of external calibration standards that are matrix matched to sample solutions containing 100 ug/g U. The NIST standard reference material U960 (U metal) is the cleanest source of U identified for matrix matching purposes. The use of two sets of calibration standards, each containing select trace elements, allows contributions from interferences to be calculated and subtracted. Interference correction is important for the measurement of accurate REE concentrations, as the REE are particularly prone to being impacted by polyatomic oxide interferences. A two-stage rinsing routine consists of 0.16M HNO3-0.01M HF then 0.32M HNO3 is used between each sample. Trace element measurements are made using a Thermo Element XR high resolution ICP-MS equipped with a cooled spray chamber. The method described provides a means for accurate and precise measurement of low abundance UOC trace elements and opens the door for discovery of hitherto unrecognized source and process signatures.

C-PCS

Name	Divina Anunciado	LA-UR 12-00125
Group:	C-PCS	
Mentor:	Dung Vu	
Field of Study:	Chemistry	
Discipline:	Biological/Biophysical Chemistry	
Appointment:	Postdoc Research Associate	
Poster Title:	Investigation of the Conformational Changes and Dynamics of Alpha-Synuclein	

ABSTRACT

The role of a-synuclein aggregation in Parkinson's disease is not fully understood. The crucial need for therapies that not just alleviate the symptoms but modify the disease rely on the better understanding of the folding, misfolding and aggregation of a-synuclein. We aim to characterize the conformations and intermediates involved in the solution state of a-synuclein. We will elucidate the molecular mechanisms involved in the folding and in the binding of this intrinsically disordered protein to different ligands at different physicochemical conditions. Finally, we hope to be able to characterize not just the folding pathway of a-synuclein but also its aggregation process.

Our approach utilizes both experimental techniques and molecular dynamics simulation. For our experimental work we use vibrational spectroscopy, circular dichroism and neutron scattering techniques. Infrared spectroscopy is sensitive to the protein's structural changes under different conditions (high temperature, low pH, with metals, with membrane). Our infrared spectroscopy and all-atom MD simulation data at different conditions show that transient structural conformations are populated. These populated states may provide some insight into the folding and aggregation of a-synuclein. In addition, our small angle neutron scattering (SANS) work has provided further details on the protein's flexibility, length and shape. Overall, any additional knowledge on the a-synuclein's molecular details of binding, folding and aggregation that we can obtain from our studies are essential to understanding its function and its role in the pathogenesis of Parkinson's disease.

Name	Heming He	LA-UR 11-07138
Groups:	C-PCS and C-NR	
Mentors:	Kirk Rector and Marianne Wilkerson	
Field of Study:	Chemistry	
Discipline:	Physical Chemistry	
Appointment:	Postdoc Research Associate	
Poster Title:	Detection of Chemical Speciation in Ultra-Thin Uranium Oxide Film	

ABSTRACT

The complexity of uranium oxide has been described as "awesome", exhibiting some of the most intriguing and challenging chemistry known. Indeed, the compositions of uranium oxides are numerically variable, and susceptible under some conditions, even the deceptively simple cubic structure of UO2 masks incredibly complex speciation following exposure to air. The scientific challenge is to identify, measure, and understand those aspects of speciation of actinide analytes that carry information about the changes within these materials as a function of aging conditions without disturbing their microstructures. Here, we demonstrate for the first time the combination of two powerful techniques, Neutron Reflectometry (NR) and Surface Enhanced Raman Spectroscopy (SERS), to nondestructively characterize the chemical speciation in ultra-thin uranium oxide films with angstrom level resolution. Our results reveal that the UOx film is composed of three sublayers: A ~38 Å thick of dense layer was formed along the UOx/substrate interface probably due to heteroepitaxial growth of the α-U3O8; The adjacent sublayer consists of a ~900 Å thick single phase of uranium oxide, which could be assigned to α-UO3; Both NR and SERS agree that the top, atmosphere-exposed, layer is γ-UO3 with a thickness of ~115 Å. The measurements establish the ability to determine the chemical speciation of both the surface and underlying layers of a film that could lead to a quantitative measure of the exposure duration of the analyte. This fundamental approach provides the ability to characterize the rates of changes in environmental samples. The practical implication of this behavior is the ability to interpret the chronometric age information within a given sample, to maintain stable forms of nuclear fuel over time, to provide safe mechanisms for storage of spent nuclear fuel, to predict transport and fate, and to assess the forensic properties of nuclear materials.

Name	Hunter McDaniel	LA-UR 12-20980
Group:	C-PCS	
Mentors:	Jeff Pietryga and Victor Klimov	
Field of Study:	Materials Science	
Discipline:	Photovoltaic Applications for Quantum Dots	
Appointment:	Postdoc Research Associate	
Poster Title:	Highly Luminescent CuInS2 Quantum Dots for Sensitized Solar Cells	

ABSTRACT

With a bulk band gaps near 1.5eV, large extinction coefficients, high carrier mobilities, and lack of toxic components, ternary chalcopyrite semiconductors such as CuInS2 have shown great promise as absorbing layers in solar cells. Utilizing nanoscale volumes of these materials (eg. colloidal quantum dots), additional advantages such as band gap tunability and solution processability can be achieved. We have shown that gram scale quantities of CuInS2 quantum dots can be synthesized with a range of sizes and band gaps with 90%+ chemical yield. By applying a mild Cd or Zn oleate treatment to the dots, their photoluminescence (PL) quantum yield increases by a factor of up to 20, approaching 100%, while the absorption is negligibly modified. High radiative quantum yields imply suppressed non-radiative recombination pathways, crucial for high efficiency photovoltaics. Electron transfer from CuInS2 to TiO2 is not hindered by the Cd/Zn treatment making these dots attractive for quantum dot sensitized solar cells. Ongoing studies into charge transport through films of CuInS2 quantum dots may lead to further insights and pave the way for solid-state photovoltaics incorporating thick enough films to appreciably absorb sunlight. In this presentation I will discuss the mechanism for enhanced PL quantum yield in treated CuInS2 quantum dots and implications for solar cell applications.

Name	Rama Murthy Sakamuri	LA-UR 12-20941
Group:	C-PCS	
Mentors:	Harshini Mukundan and Basil Swanson	
Field of Study:	Bioscience	
Discipline:	Biology	
Appointment:	Postdoc Research Associate	
Poster Title:	GO FISH: Capturing of Viable Bacteria using Surface Bound Siderophores	

ABSTRACT

Detection of viable bacteria is a challenge in variety of fields like clinical diagnosis, food industry and environmental monitoring. The conventional microbiological detection methods like culturing, nucleic acid and antibody-based techniques are either time consuming or labor intensive and sometimes cannot discriminate between viable bacteria over debris. Herein we report a selective detection method to identify only viable bacteria in complex matrices, and discriminate them from their dead counterparts using bacterial siderophores (SDPs). Bacteria acquire iron from its environment by releasing iron chelators known as SDPs, the iron-bound SDPs are subsequently internalized. This is a highly conserved process that occurs only in intact bacteria. The SDP, Desferrioxamine B (Desf B) was tethered to a glass slide and is used to specifically capture viable bacteria from a mixture of viable and dead *Escherichia coli*, as demonstrated by fluorescence microscopy. We have used both direct and biotin-avidin conjugation strategies to tether Desf B on to the glass slides functionalized with silane-based self-assembled monolayers. Both of the approaches were successful in the said goal, however direct conjugation strategy yielded less non-specificity. We have also analyzed the density of images obtained upon fluorescence staining using edge detection with a Canny edge detector. This novel application of a software analysis tool originally developed for satellite imaging to biological staining allows for accurate quantitation of observed data.

Name	John Stewart	LA-UR 12-21024
Group:	C-PCS	
Mentor:	Victor Klimov	
Field of Study:	Chemistry	
Discipline:	Physics/Spectroscopy	
Appointment:	Director's Postdoc Fellow	
Poster Title:	Shape and Composition Effects on Carrier Multiplication Efficiency in PbX Salts	

ABSTRACT

In this talk I will present recent results of a collaborative effort investigating the effects of shape and composition on the quantum efficiency of carrier multiplication (CM) in lead salt nanocrystals. These materials are promising candidates for exploring generation-III photovoltaic concepts that rely on CM, the process in which a single photon generates more than one electron-hole pair. While CM is a promising mechanism for efficient charge generation, it is still not very well understood. To this end, we investigate the role that composition can play in determining the efficiency of carrier multiplication. Despite the many apparent similarities of PbS, PbSe and PbTe in their bulk form, we find that these compounds exhibit strikingly different CM yields in their nanocrystalline form. We suggest that the difference in CM yields in these nanomaterials highlight the importance of competing relaxation mechanisms, such as phonon emission. Additionally, motivated by recent theoretical efforts, we investigate the importance of shape effects on carrier multiplication. We find that dimensionality plays an important role in carrier-carrier interactions as evidenced by its effect on Auger recombination rates and CM yields. These results should prove useful for predicting future materials and shapes to investigate for increasingly high CM yields.

Computer, Computational, and Statistical Sciences Division
CCS-2

Name	Guillaume Simon	LA-UR 12-20966
Groups:	CCS-2 and T-3	
Mentors:	Balu Nadiga and Phil Jones	
Field of Study:	Earth, Atmospheric, and Ocean Sciences	
Discipline:	Stratified Rotation Turbulence	
Appointment:	Postdoc Research Associate	
Poster Title:	Interactions between Balanced and Unbalanced Homogeneous Turbulent Cascades; or How Ocean Circulation Equilibrates	

ABSTRACT

Submesoscale processes are distinguished by order-one Rossby and Richardson numbers with typical size of O(1-10km) in the ocean. The dynamics of submesoscale processes are distinct from those of the largely quasi-geostrophic mesoscale (typical size of O(10-100km)) and fully three-dimensional small processes (size less than 100m). While it's known that submesoscale turbulence arises from frontogenesis due to mesoscale strain and submesoscale instabilities, an understanding of their influence on large-scale circulation is only nascent. We focus on their role in mediating energy exchanges between the larger scale,balanced, circulations and smaller scale, fully-unbalanced three dimensional processes.

A computational challenge in this project is the simultaneous and proper simulation of a range of scales ranging from the balanced mesoscales down to the unbalanced scales, still well removed from the regime of full three dimensional turbulence.

We use a tree periodic Boussinesq-Coriolis model in a range of parameters compatible with the Southern Ocean Circulation. First, the initial value problem leading to large Richardson number baroclinic instabilities will be presented. Next, the long range statistically stationary state will be analyzed.

CCS-3

Name	Rafael Zárate-Miñano	LA-UR 12-20845
Group:	CCS-3	
Mentor:	Marian Anghel	
Field of Study:	Engineering	
Discipline:	Power Systems	
Poster Title:	Wind Speed Model for Power System Dynamic Analysis	

ABSTRACT

A continuous-time wind speed model based on stochastic differential equations is proposed. The model is intended to generate wind speed trajectories with statistical properties similar to those observed in the wind speed historical data available for a particular location. The proposed model is parsimonious in the sense that it only uses the information about the marginal distribution and the autocorrelation observed in the wind speed data. Since the model is continuous, it can be used to simulate wind speed trajectories at different time scales. However, the model is designed for being used in power system dynamic simulations, i.e., in the time frame of seconds.

DECISION APPLICATIONS DIVISION
D-4

Name	Annarita Giani	LA-UR 12-20828
Groups:	D-4 and T-4	
Mentors:	Russell Bent and Michael Chertkov	
Field of Study:	Engineering	
Discipline:	Power Systems	
Appointment:	Director's Postdoc Fellow	
Poster Title:	Smart Grid Attack Characterization and Countermeasures	

ABSTRACT

In this talk we concentrate on data integrity attacks to power grid data. Real power injections at loads and generators, and real power flows on selected lines in a transmission network are monitored, transmitted over a SCADA network to the system operator, and used in state estimation algorithms to make dispatch, re-balance and other energy management system [EMS] decisions. Coordinated cyberattacks of power meter readings can be arranged to be undetectable by any bad data detection algorithm. These unobservable attacks present a serious threat to grid operations. Of particular interest are sparse attacks that involve the compromise of a modest number of meter readings.

The contribution of our work is the following. In the special circumstance where all lines are metered, we derive canonical forms for 3, 4, and 5-sparse unobservable attacks in terms of the graph of the power network. And, given a power network, we offer an algorithm to find them.

We next consider the problem of using known-secure PMUs to thwart an arbitrary collection of cyberattacks. We offer a characterization of buses at which these PMUs must be placed to mitigate the collection of attacks. Finding the minimum number of necessary PMUs is NP-hard. We show that it is sufficient to place p+1 PMUs at carefully chosen buses to neutralize a collection of p cyberattacks.

Earth and Environmental Sciences Division
EES-14

Name	Allison Aiken	LA-UR 12-20043
Groups:	EES-14 and ISR-2	
Mentors:	Manvendra Dubey and Petr Chylek	
Field of Study:	Earth and Space Science	
Discipline:	Atmospheric Chemistry	
Appointment:	Director's Postdoc Fellow	
Poster Title:	Black Carbon: Ambient Intercomparisons of Physical and Optical Properties	

ABSTRACT

Currently, absorbing aerosols are thought to be the most uncertain factor in atmospheric climate models (~0.4–1.2 W/m2), and potentially the second most important factor after CO2 in global warming (1.6 W/m2; Ramanathan and Carmichael, Nature Geoscience, 2008; Myhre, Science, 2009). While most well-recognized atmospheric aerosols, e.g., sulfate from power plants, have a cooling effect on the atmosphere by scattering solar radiation, black carbon (BC or "soot") absorbs sunlight strongly, which results in a warming of the atmosphere. Direct online measurements of BC are made with the Single Particle Soot Photometer (SP2), which detects BC by incandescence from individual particles. Measurements from the SP2 are combined with absorption measurements from the three-wavelength photoacoustic soot spectrometer (PASS-3) at 405, 532, and 781 nm and the ultraviolet photoacoustic soot spectrometer (PASS-UV) at 375 nm to determine wavelength-dependent mass absorption coefficients (MACs) and absorption angstrom exponents (AAEs), among other optical properties. Ambient measurements of different BC types were collected during three different campaigns. (1) High mass concentrations of biomass burning were sampled during the Las Conchas fire, the largest wildfire in New Mexico history that started in the Jemez Mountains in Northern New Mexico and burned over 100,000 acres during the summer of 2011. (2) Low mass concentrations of aged transported "background" pollution were sampled during BEACHON-RoMBAS (Bio-hydro-atmosphere interactions of Energy, Aerosols, Carbon, H2O, Organics & Nitrogen – Rocky Mountain Biogenic Aerosol Study), a field campaign that was located in the Manitou Forest Observatory near Colorado Springs, Colorado, in summer 2011. (3) Fresh highway, aged outflow, and wood-burning BC types were sampled during the ClearfLo (Clean Air for London) campaign in Detling, England, during winter 2012. Optical properties are compared from these different BC types and compared with laboratory measurements, and size-resolved information is used to predict the absorptive effects of these climate-relevant aerosols on our atmosphere.

Name	Michael Cheshire	LA-UR 12-20906
Group:	EES-14	
Mentor:	Florie Caporuscio	
Field of Study:	Earth, Atmospheric, and Ocean Sciences	
Discipline:	Geochemistry and Clay Mineralogy	
Appointment:	Postdoc Research Associate	
Poster Title:	Hydrothermal Alteration of a Bentonite-Metal Engineered Barrier System at 150 Bar and up to 300 C Under Brine Conditions	

ABSTRACT

The United States recently has initiated the Used Fuel Disposition (UFD) campaign to evaluate various geological repository settings due to the closure of the Yucca Mountain project. Researchers that are part of the UFD campaign are presently evaluating generic options for the disposal of high-level, spent nuclear fuel within repositories ranging from mine to deep borehole settings. Previous work describing Engineered Barrier Systems (EBS) for repositories has focused on low temperature and pressure conditions. The focus of this experimental work is to characterize the stability and alteration of a bentonite-based EBS with different waste container materials in brine at higher heat loads and pressures.

Bentonite used in the experiments is primarily a Na-montmorillonite from Colony, Wyoming. The experimental mixtures were 1) brine–clay, 2) brine–clay–304 stainless steel(304SS), 3) brine–clay–316 stainless steel (316SS), and 4) brine–clay–copper, with a brine/bentonite ratio of 9-10. Each experiment was buffered at the magnetite-iron oxygen fugacity univarient curve using Fe3O4 and Fe filings. A Na-Ca-K-Cl-based brine consisting of 1934 ppm total dissolved solids at a pH of 8.6 was used as the brine material. All experiments were run at ~150 bar and 125 to 300 C for one month. Liquid samples during the experiment were extracted to monitor changes in water chemistry and analyzed with inductively coupled plasma-mass spectrometry. The pre- and post-reaction solid phases were analyzed via X-ray diffraction and analytical electron microscopy.

No smectite illitization was observed in these reactions. However, it appears that K-smectite was produced possibly providing a precursor to illitization. It is unclear if the reaction times were sufficient for the bentonite illitization at 212 and 300 C or the conditions for illite formation were obtained. The more notable clay mineral reactions occur at the brine/304SS boundary. Authigenic chlorites and smectites (possibly Fe-rich saponite or nontronite) formed a thin layer on the 304SS plate surface. Chlorite formation was not observed in the brine-bentonite experiments, suggesting chlorite growth is associated with the 304SS surface. Partial dissolution of the 304SS is most likely the Fe2+ source in the chlorite formation; however, dissolution of the Fe/Fe3O4 filings could also be the Fe2+ source with 304SS plates acting as a substrate for chlorite growth.

There appears to be no significant mineralogical changes away from the steel-smectite interface. This research has shown that the waste container will act as a substrate for mineral growth in response to corrosion. However, it is presently unknown if the chlorite and Fe-rich smectite will act as a passivating agent or if their presence will facilitate further corrosion of the waste containers. The role of these Fe-rich minerals on the stability of steel canisters at elevated heat loads is currently under investigation. Mineral growth on the waste container is influence by the container, buffer, and brine composition in addition to the pressure and temperature conditions of the repository.

Name	Chandana Gangodagamage	LA-UR 11-11184
Groups:	EES-14 and ISR-3	
Mentors:	Cathy Wilson and Steven Brumby	
Field of Study:	Earth, Atmospheric, and Ocean Sciences	
Discipline:	Civil Engineering	
Appointment:	Postdoc Research Associate	
Poster Title:	Topographic Signature of Climate Change	

ABSTRACT

Since the Last Glacial Maximum (LGM), glacier in North America has declined across the landscape crono-sequentially from 19-10 ka BP; subsequent exposure to the warmer interglacial climatic conditions for the last Holocene makes the continental landscape an ideal baseline setting to test the different landscape evolution trajectories in real climatic and environmental conditions. As glacial retreats, warmer interglacial climate driven fluvial erosion and hillslope mass wasting processes supplanted the glacial processes, but the rate of denudation primarily driven by the postglacial in-situ climatic exposure. The landscape on the north side of the Laurentide ice sheet exposed to much colder climate conditions (< 0 0C) facilitates the permafrost landscape, where mass wasting process primarily driven by seasonal freeze–thaw, resulted a rudimentary channel network, still preserves substantial glacial signature.

The landscape on the south side of the Laurentide ice sheets exposed to moderate cold climatic conditions, where no permafrost was supported, shaped by the fluvial erosions and hillslope diffusion has developed more temperate landscape features while preserving some glaciated signature; Based on our landscape analysis, we show that the topographic denudation on these landscapes over the past Holocene has imprinted a unique climatic signature that can be captured from high resolution Digital Elevation Model (DEM ~ 1m) data; major differences are in landscape regime and regime transitions; glaciated permafrost landscapes are primarily characterized by narrow divergent hilltops (< 15 m), longer convergent flow paths (~600-1000 m) in hillslopes, and abrupt hillslope to fluvial transitions (< 100 m); glaciated no-permafrost landscape characterized by relatively large divergent hillslopes (~ 30-100 m), moderately long convergent flowpaths (400-500 m), and hillslope to fluvial transition through longer networks hollows (300-1000 m). We demonstrate our findings using high resolution lidar dataset obtained for Trail Valley, Mackenzie River, Canada; Brooks Range, North Slope, Alaska; Tenderfoot Creek, Montana, and Pleasant, Maine, USA that were previously occupied by North American Laurantide ice sheet and Brooks Range glaciers. South Fork Eel River, California is used as a representative temperate basin.

Name	Peng He	LA-UR 12-20926
Group:	EES-14	
Mentor:	Amr Abdel-Fattah	
Field of Study:	Earth, Atmospheric, and Ocean Sciences	
Discipline:	Microfluidics, Colloidal and Interface Science	
Appointment:	Postdoc Research Associate	
Poster Title:	Microfluidics into the Underground	

ABSTRACT

Increasing global carbon emissions from burning fossil fuels are detrimental to the environment and evidently responsible for undesired global climate changes and extreme weather. A proposed solution to reduce atmospheric CO2 concentration is to capture the emission from power plants into liquid form and inject it into deep underground porous geologic formations for permanent storage. One of the challenges of this scheme is CO2 leakage into the surrounding aquifer or back to the atmosphere. Understanding of multiphase flow involved in replacement of brines by CO2 and capillary trapping inside in the porous rocks are keys to a successful CO2 sequestration operation, and current understanding of such complex processes under relevant conditions is immature. Microscale experiments were performed to reveal the fundamental mechanisms underlying such processes. We utilized direct visualization geomimitic systems in which a wetting phase (oil) is displaced by a non-wetting phase (water) at different Ca and mobility rations to understand the following interfacial phenomena: 1) flow patterns evolving of water fingering into oil (to mimic CO2 replacing brine); 2) capillary trapping of residual fluids; and 3) the impact of adjusting the surface properties and porosity of the microfluidic module representing various rock conditions. In this showcase, I will also demonstrate an on-going construction and testing of a unique high-pressure, high-temperature (high P-T) microfluidic facility, and discuss preliminary results on quantifying the above mentioned interfacial phenomena under high P-T conditions, and incorporating experiment results with a state-of-the-art lattice Boltzmann simulations.

A second effort of my research is to extend my PhD research in hydrogels to develop a technology for sealing subsurface CO2 leakage and encapsulation microalgae cultivation for biofuel applications.

Name	Rodica Lindenmaier	LA-UR 12-20907
Groups:	EES-14 and ISR-2	
Mentors:	Manvendra Dubey, Bradley Henderson, and Steven Love	
Field of Study:	Earth, Atmospheric, and Ocean Sciences	
Discipline:	GHG Emissions, Pollution, Air Quality	
Appointment:	Postdoc Research Associate	
Poster Title:	Four Corners - LANL 125HR Measurements of GHGs and Pollutants for Climate and Air Quality	

ABSTRACT

There is strong evidence that surface warming observed since 1900 goes beyond natural climate variability, with most of it due to human activities. However there is significant uncertainty in predicting GHG concentrations as future climate changes can amplify natural net GHG fluxes from forests, agriculture and soils, particularly in the Arctic that is warming dramatically. A future climate treaty would also require methods to verify GHG emissions from power plants and urban areas that do not exist, and are challenging since the signals are relatively small due to high and variable backgrounds. Novel strategies, such as measurements of co-emitted pollutants TGs that have high signals and low backgrounds are needed to predict GHG-climate feedbacks and verify national emissions. My observations were made at the Four Corners site, close to two power plants: San Juan and Four Corners. Results of the LANL Bruker 125HR Fourier transform spectrometer will be presented.

EES-16

Name	Satish Karra	LA-UR 12-20985
Group:	EES-16	
Mentors:	Qinjun Kang and Scott Painter	
Field of Study:	Engineering	
Discipline:	Mechanical Engineering	
Appointment:	Postdoc Research Associate	
Poster Title:	Massively Parallel Computations to Simulate Earth's Permafrost Dynamics	

ABSTRACT

Degradation of the near-surface permafrost layer due to changes in the climate is known to impact the hydrological, ecological and the biogeochemical responses in the ground. From a hydrological perspective, it is important to understand the movement of the various phases of water (gas, liquid and ice) during the freezing and thawing of this permafrost layer. In this work, we present a new non-isothermal, single-component (water), three-phase formulation which treats air as an inactive component. This formulation is different from the recently proposed two-component, three-phase formulation by Painter (2011) that has been used to model permafrost dynamics in Earth and formation and evolution of a planetary-scale cryosphere on Mars. The new formulation is implemented in the massively parallel sub-surface flow and reactive transport code PFLOTRAN that has been developed as part of the SciDAC-2 project at LANL.

Validation studies using previously published experimental data are performed. Three-dimensional simulations of the permafrost freezing and thawing due to seasonal variation are also presented.

EES-17

Name	Brian Anderson	LA-UR 12-20815
Group:	EES-17	
Mentors:	Timothy Ulrich and Pierre-Yves Le Bas	
Field of Study:	Physics	
Discipline:	Acoustics and Nondestructive Evaluation	
Appointment:	Postdoc Research Associate	
Poster Title:	Time Reversal Techniques to Localize and Characterize Damage in Solid Structures	

ABSTRACT

Time reversal is a method of focusing wave energy to a specific location in space and/or to locate an unknown source of wave energy. When elastic waves of sufficient amplitude impinge upon a crack in a solid structure, it can cause the crack to vibrate in a nonlinear fashion. In other words, if the two surfaces of a crack vibrate with large enough amplitude they can come in contact with each other and therefore locally distort the vibrations as they pass through the crack. For example if a crack is vibrated with a sine wave at a single frequency with large enough amplitude to induce clapping of the crack then harmonics of this sine wave frequency are generated. We use time reversal as a method to induce a localized focusing of energy at various locations to look for harmonic signatures, which indicates cracking locations, even when these cracks may not be visible. We can also use these techniques to inspect two laminated plates for locations where the two plates are not bonded properly. This presentation will illustrate the abilities of the time reversal process to focus wave energy in an elastic solid and provide examples of locating cracks using this process. The results are from experiments conducted on various solid samples, such as glass and aluminum, using piezoelectric transducers and scanning laser vibrometers.

Name	Eric Daub	LA-UR 12-10416
Groups:	EES-17 and T-CNLS	
Mentors:	Paul Johnson, Jim TenCate, and Robert Ecke	
Field of Study:	Physics	
Discipline:	Geophysics, Condensed Matter, Materials Science	
Appointment:	Postdoc Research Associate	
Poster Title:	Are Megaquakes Clustered?	

ABSTRACT

We study statistical properties of the number of large earthquakes over the past century. We analyze the cumulative distribution of the number of earthquakes with magnitude larger than threshold M in time interval T, and quantify the statistical significance of these results by simulating a large number of synthetic random catalogs. We find that in general, the earthquake record cannot be distinguished from a process that is random in time. This conclusion holds whether aftershocks are removed or not, except at magnitudes below M = 7.3. At long time intervals (T = 2-5 years), we find that statistically significant clustering is present in the catalog for lower magnitude thresholds (M = 7-7.2). However, this clustering is due to a large number of earthquakes on record in the early part of the 20th century, when magnitudes are less certain.

Name	Youzuo Lin	LA-UR 12-20960
Group:	EES-17	
Mentor:	Lianjie Huang	
Field of Study:	Earth, Atmospheric, and Ocean Sciences	
Discipline:	Geophysics	
Appointment:	Postdoc Research Associate	
Poster Title:	Quantitative Geophysical Monitoring of Enhanced Geothermal Systems	

ABSTRACT

Quantitative geophysical monitoring of enhanced geothermal systems (EGS) plays a key role in optimizing geothermal energy production. Waveform inversion of time-lapse seismic data is a quantitative monitoring approach. The traditional Tikhonov regularization used in waveform inversion tends to smooth reconstruction results and gives inaccurate values of changes of geophysical properties within EGS reservoirs. We develop a new double-difference elastic-waveform inversion method with a modified total-variation regularization scheme to improve the quantification of EGS reservoir changes. The double-difference elastic-waveform inversion method inverts for reservoir changes utilizing differences of time-lapse seismic data. The modified total-variation regularization improves not only the reconstruction of the baseline model, but also reservoir changes, particularly in small regions within EGS reservoirs. We use synthetic time-lapse seismic data for a Brady's EGS model to verify our new method. Our numerical results clearly demonstrate that our double-difference elastic-waveform inversion with a modified total-variation regularization scheme is a promising tool for quantitative monitoring of EGS reservoirs.

Name	Jian Zhang	LA-UR 12-20882
Group:	EES-17	
Mentors:	Xiaoning Yang and William Phillips	
Field of Study:	Earth, Atmospheric, and Ocean Sciences	
Discipline:	Seismology	
Appointment:	Postdoc Research Associate	
Poster Title:	Daylight Imaging with Seismic Noise	

ABSTRACT

Traditionally our understanding of Earth's interior has largely come from seismic imaging using earthquakes. Seismic noise, namely Earth's background vibrations, is usually disregarded or suppressed. In recent years, seismologists have revealed that correlation of seismic noise recorded at two locations can provide the so-called "Green's function" between the two locations, which contains Earth properties such as seismic wave velocity, density, and attenuation. This "daylight imaging" technique, in analogy to the illumination of shaded areas by scattered daylight, has opened up the use of ubiquitous seismic noise as a new dataset for Earth science studies, especially in regions where earthquakes are scarce.

Many studies have demonstrated great success of daylight imaging in extracting seismic velocity. However, imaging Earth's attenuation (i.e., how energy decays in the Earth) with seismic noise remains a challenge, as the amplitude of empirical Green's functions from noise is often biased due to uneven distribution of seismic noise. In this work we use seismic noise recorded by the USArray stations to explore novel techniques that may advance daylight imaging of Earth's attenuations. We find that three processing procedures, i.e., (**1**) temporal flattening, (**2**) temporal stacking, and (**3**) correlation of the coda of correlation (C^3), may be used to reduce bias and allow us to obtain a more reliable attenuation estimate.

High Performance Computing Division
HPC-5

Name	Adam Manzanares	LA-UR 12-20021
Group:	HPC-5	
Mentors:	Michael Lang, John Bent, and Meghan Wingate	
Field of Study:	Mathematics and Computer Science	
Discipline:	Computer Science	
Appointment:	Metropolis Postdoc Fellow	
Poster Title:	PLFS - A Transformative I/O Middleware Layer	

ABSTRACT

Extracting high data bandwidth and metadata rates from parallel file systems is notoriously difficult. User workloads almost never achieve the performance of synthetic benchmarks. The reason for this is that real-world applications are not as well-aligned, well-tuned, or consistent as are synthetic benchmarks. There are at least three possible ways to address this challenge: modification of the real-world workloads, modification of the underlying parallel file systems, or reorganization of the real-world workloads using transformative middleware. This poster documents the challenges and successes of the Parallel Log Structured File System, a transformative I/O middleware layer developed at Los Alamos. PLFS is envisioned as part of the Exascale stack due to its high performance and flexibility.

LANL Institutes Office
INST-OFF

Name	Steven Anton	LA-UR 12-21017
Groups:	INST-OFF and AET-1	
Mentor(s):	Charles Farrar and Kevin Farinholt	
Field of Study:	Engineering	
Discipline:	Mechanical Engineering	
Appointment:	Postdoc Research Associate	
Poster Title:	Piezoelectret Foam-Based Vibration Energy Harvester for Low-Power Energy Generation	

ABSTRACT

Harvesting ambient energy to supply power to low-power electronics, such as wireless sensors, has gained tremendous interest in the research community in the last decade. Several modes of energy harvesting have been investigated including the scavenging of solar, thermal, wind, and vibration energy. A significant amount of research has focused on vibration-based energy harvesting using electrostatic, electromagnetic, and piezoelectric transduction mechanisms. In this work, vibration energy harvesting using piezoelectret foam, a novel type of piezoelectric material, is investigated. Piezoelectrets are made from foamed polymers (typically polypropylene) in which electric charge is permanently deposited onto the surfaces of the internal voids in the structure, thus creating macroscopic dipoles that facilitate piezoelectric response. Energy is generated in response to thickness changes in the material which primarily cause changes in the charged air voids, which act as parallel plate capacitors. A schematic showing the construction and piezoelectric response of piezoelectret foams is given in Figure 1. The ability of flexible piezoelectric materials, such as piezoelectret foam, to conform to curved and irregular surfaces is advantageous over conventional piezoceramics, which are limited to applications containing flat mounting surfaces. The appeal of piezoelectrets over conventional piezoelectric polymers, such as polyvinylidene fluoride (PVDF), is their large piezoelectric d33 coefficient. Piezoelectrets can exhibit d33 up to 250 pC/N, which is 7 times larger than that of PVDF (-33 pC/N). A larger piezoelectric coefficient signifies the ability to more freely convert mechanical energy into electrical energy. Additionally, the density of piezoelectret foam is significantly less than that of piezoceramics and PVDF, therefore, it carries a much smaller weight penalty when added to mass-critical systems.

This work presents an investigation of low-level energy harvesting using piezoelectret material. Basic details of the fabrication of piezoelectrets and the transduction principles of the material are first given. Next, a review of previous work by the authors investigating the mechanical (tensile) properties and electromechanical response of piezoelectret materials is presented. Details of the design and fabrication of a piezoelectret energy harvester are outlined. From the author's previous work, it has been concluded that the voltage output of piezoelectret foams can be quite low under modest excitation (around 0.1 V for excitation of a 6.5 cm2 sample), therefore, an energy harvester design is proposed in which larger samples are utilized in an effort to increase the voltage output to a useable level. A simple energy harvesting circuit is developed in which the sinusoidal voltage output of the piezoelectret harvester is conditioned in attempt to provide stable DC power for low-power electronics. Comparisons are made between the performance of piezoelectret foams and conventional piezoelectric ceramics and piezoelectric polymer materials and conclusions are drawn about the use of piezoelectret foam as a material for low-level vibration harvesting.

Name	Steven Anton (continued)	LA-UR 12-21017
Groups:	INST-OFF and AET-1	
Mentors:	Charles Farrar and Kevin Farinholt	
Field of Study:	Engineering	
Discipline:	Mechanical Engineering	
Appointment:	Postdoc Research Associate	
Poster Title:	Piezoelectret Foam-Based Vibration Energy Harvester for Low-Power Energy Generation	

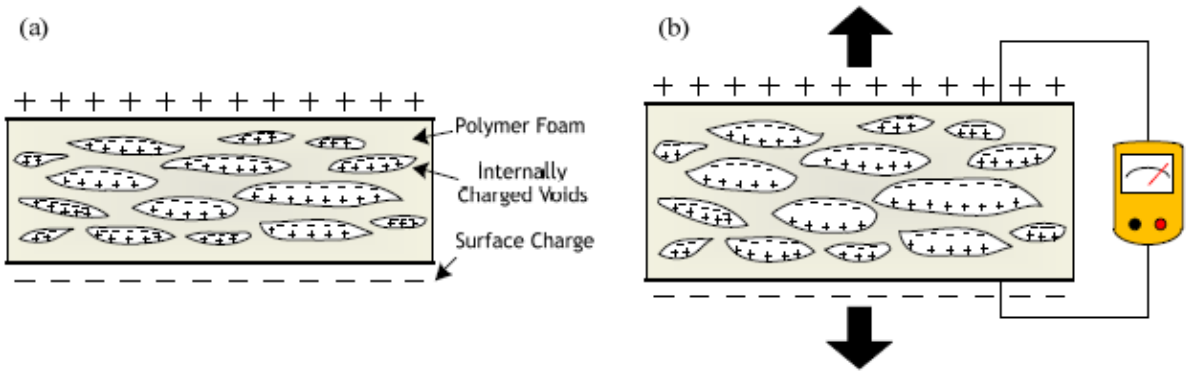


Figure 1. (a) Cross-sectional schematic of and (b) representation of piezoelectricity in piezoelectret foams.

International, Space, and Response Division
ISR-1

Name	Brent Budden	LA-UR 12-00354
Group:	ISR-1	
Mentors:	Marc Kippen, Laura Stonehill, and Richard Schirato	
Field of Study:	Physics	
Discipline:	Radiation Detection, Image Reconstruction	
Appointment:	Postdoc Research Associate	
Poster Title:	Characterization of Cs2LiYCl6:Ce3+ (CLYC) Scintillation Waveforms under Gamma- and Neutron-induced Excitation	

ABSTRACT

Cs2LiYCl6:Ce3+ (CLYC) is a promising new inorganic scintillator for gamma and neutron detection. It emits at a peak wavelength of 373 nm (well-matched to many commercial photomultiplier tubes), has a density of 3.31 g/cm3, and provides better energy resolution than commonly-used NaI crystals. CLYC provides thermal neutron sensitivity by means of the 6Li(nth,α)t reaction with Q-value of 4.78 MeV (quenched to gamma-equivalent energy of about 3.5 MeV).

As with other doped elpasolites, CLYC exhibits primarily three scintillation mechanisms under x-ray/gamma-ray excitation with a range of decay times: emission by self-trapped excitons (STEs, slow), binary Vk and electron diffusion (intermediate), and direct electron-hole capture by Ce3+ trivalent doping ions (fast). A fourth mechanism, core-to-valence luminescence (CVL), is an ultrafast emission reportedly observed in CLYC under gamma-excitation. The absence of CVL in waveforms from thermal neutron excitation enables the implementation of pulse-shape discrimination to distinguish gammas from neutrons. CLYC is therefore a suitable alternative to He3 tubes, which are commonly used in neutron detection applications.

The exact combination of scintillation mechanisms responsible for CLYC's optical emission and its ability to discriminate between gamma and thermal neutrons is debated in the literature. We therefore investigate the shape of the CLYC waveforms at room temperature with a fast waveform digitizer. Compound exponential fits to these data provide decay times which are correlated to those previously-published to verify which mechanisms contribute to the emission. Under gamma excitation, we observe the fast, intermediate, and slow emission decays reported previously, and we see evidence of CVL. Thermal neutron waveforms exhibit intermediate and slow decays, but show no evidence of fast or ultrafast emission.

To further characterize CLYC emissions, we apply the same measurements at a range of temperatures: from -20 to 50° C. Exponential fits to these data indicate that the relative efficiencies of the scintillation mechanisms are strongly dependent on temperature; intensity from Vk diffusion is enhanced, while Ce3+ transitions and STE emissions are suppressed. Apparent waveform shapes thus change significantly, though the continued absence of the fast/ultrafast emission in neutron waveforms means PSD is feasible with CLYC even at these thermal extremes.

Name	Raluca Ilie	LA-UR 12-20618
Groups:	ISR-1 and ISR-DO	
Mentors:	Ruth Skoug and Herb Funsten	
Field of Study:	Earth, Atmospheric, and Ocean Sciences	
Discipline:	Space Science	
Appointment:	Postdoc Research Associate	
Poster Title:	Global View of Inner Magnetosphere Composition during Magnetic Storms	

ABSTRACT

The presence of oxygen, although short lived, in the inner magnetosphere has been known for quite some time. Its relatively short life compared to the hydrogen ions is mainly due to the significantly larger O+/H charge exchange cross section as well to the fact that O+ is efficiently lost to the atmosphere by pitch-angle scattering.

Variations in the ion composition of the inner magnetosphere alter the dynamics of the plasma by changing the average lifetime of particle population. Although the ratio of hydrogen to oxygen has been shown to be highly dependent on geomagnetic activity, a global view of the oxygen injection is not yet possible to obtain using observations only. Therefore the timing and the injection mechanisms as well as the loss of O+ from the ring current are still subject to debate.

The TWINS ENA imagers can distinguish between the major ion constituents of the ring current, providing a new capability for studying the composition of the ring current. Combining TWINS images with modeling of the global magnetosphere opens up the possibility for global viewing of ring current composition. Simulations using the Space Weather Modeling Framework (SWMF) involving composition measurements from TWINS are used to investigate the global dynamics and energization of ions throughout the whole magnetosphere and to address the impact of inner magnetosphere ion composition on the physical processes that dominate this region.

Name	Yiqun Yu	LA-UR 12-20977
Group:	ISR-1	
Mentors:	Josef Koller, Vania Jordanova, and Sorin Zaharia	
Field of Study:	Earth, Atmospheric, and Ocean Sciences	
Discipline:	Magnetospheric Physics	
Appointment:	Director's Postdoc Fellow	
Poster Title:	The Effect of Magnetopause Shadowing on Radiation Belt Dropouts	

ABSTRACT

The energetic electron flux in the inner magnetosphere drops dramatically during geomagnetic storm events. The cause of such dropouts has been extensively investigated but remains far from well understood. The magnetopause shadowing is among the proposed mechanisms for the loss of energetic electrons. This project employs a 1D radiation belt model and investigates the contribution of the magnetopause shadowing to the observed dropout obtained by superposing electron flux from more than 100 high-speed solar-wind stream (HSS) events. Results indicate that the loss from magnetopause together with its directly induced radial diffusion can only account for 5% -30% of the observed dropouts. The range of percentages varies as a result of different magnetospheric magnetic field models, another example of the uncertainty involved in most of the work in the community that depends on the accuracy of the field model.

ISR-2

Name	Jonathan Cook	LA-UR 12-20978
Groups:	ISR-2 and ISR-4	
Mentors:	David Thompson and Joseph Palmer	
Field of Study:	Engineering	
Discipline:	Imaging Optical Detectors	
Appointment:	Postdoc Research Associate / Previous DCI PD Fellow	
Poster Title:	Properties and Capabilities of a Low-Light Imaging Detector using a Crossed-Strip Anode	

ABSTRACT

With the goal of developing a next-generation low-light imaging system capable of measuring scenes with a higher photon flux than current generation sensors can handle while maintaining high time and spatial resolution, the capabilities of a new type of sensor have been examined. The current generation of low-light imaging systems developed at LANL uses a sensor consisting of a photocathode backed by a three-layer microchannel plate and a crossed-delay line anode. A photon incident on the photocathode produces an electron, which is multiplied by the microchannel plate stack, causing a cloud of electrons to fall onto the anode. The time difference between the charge pulses reaching each side of the anode provides the location of the incident photon. Two characteristics of this configuration limit the incoming photon rate to about 1 MHz. First, there is global photon rate limit created by the need to wait for the charge pulses to reach the edge of the sensor before another photon can arrive, and, second, there is a local photon limit presented by the need for the microchannel plate to recharge after each photon, which leads bright sources to appear as dark areas. To surpass these limitations, LANL has been working with the Space Science Laboratory at University of California Berkeley to develop an improved sensor with a crossed-strip (XS) anode capable of accepting 100 times as many photons. This XS sensor has a two-layer microchannel plate stack, which has a lower gain and therefore is less susceptible to dead areas. However, the defining characteristic of the XS sensor is the anode: 32 metal strips on two axes. The upper axis has gaps between the strips, exposing the lower strips to the charge cloud pulse produced by the microchannel plate. Measuring the amount of charge that falls onto each strip creates a profile of the charge cloud along the two axes, from which the photon's position can be determined without the need to wait for the charge to move through a delay line. Using a development sensor lacking a photocathode, various properties of the sensor have been measured, including the pulse-shape and time-of-arrival variation across the anode. The charge-cloud shape has been measured and compared to literature, and the effort to improve the analysis to reach the minimum possible uncertainty in the photon position and time is ongoing with the goal of achieving 20-micron FWHM spatial resolution and sub-nanosecond time resolution. The properties and capabilities of the XS sensor will be presented.

Los Alamos Neutron Science Center
LANSCE-LC

Name	Sylvia Ann Junghans	LA-UR 12-20844
Group:	LANSCE-LC	
Mentor:	Jarek Majewski	
Field of Study:	Materials Science	
Discipline:	Soft Matter/Biophysics	
Appointment:	Postdoc Research Associate	
Poster Title:	Novel Materials for Cell Studies and Harvesting	

ABSTRACT

Controlling cell growth on different surfaces is crucial for many applications. For instance after surgery, unspecific adhesion on exogenous materials can lead to fouling that may result in infections. On the other hand, fast attachment of tissue cells is pivotal for the healing process. Hence, specific regulation of cell adhesion to substrates is a significant task especially in the biomedical field.

It has long been known that surface conditions like topology/roughness, wettability, charge, etc. are major factors in cell adhesion on various synthetic materials including Polytetrafluoroethylene, titanium or silicone. However, the literature is sparse on studies of cell growth on medical relevant substrates.

We investigated the growth of different cells types on polyelectrolyte (PE) multilayers with and without lipid bilayers deposited and could observe confluence and multiplication of cells on both substrate types. Our neutron reflectometry studies of lipid bilayers deposited on polyelectrolyte multilayer showed that the size of the water gap between the lipid bilayer and the PE covered substrate can be influenced by the environmental conditions, e.g. the pH of the surrounding medium. In principal, this “floating” of a lipid bilayer can also be applied for growing monolayer of cells and detaching them by an environmental change. Such a fabrication would simplify cell growing and harvesting for various medical application, e.g. tissue engineering.

Our approach for the fabrication of cellular monolayers that are easy to detach and transfer, creating free-floating sheets of cells also enables us to study those structures more conveniently and under in-situ conditions using neutron scattering.

Name	Graham King	LA-UR 12-20691
Group:	LANSCE-LC	
Mentor:	Anna Llobet-Megias	
Field of Study:	Chemistry	
Discipline:	Inorganic Solid State	
Appointment:	Postdoc Research Associate	
Poster Title:	Monitoring Shifts in Valence States in AMn0.5Ru0.5O3 Perovskites Using Reverse Monte Carlo Modeling of Pair Distribution Function Data	

ABSTRACT

The local structures of six perovskite compounds containing equal amounts of manganese and ruthenium on the B-site have been investigated by neutron and X-ray pair distribution function analysis. The compounds SrMn0.5Ru0.5O3, Sr0.5Ca0.5Mn0.5Ru0.5O3, and CaMn0.5Ru0.5O3 were studied to investigate the effects of pure chemical pressure on the local structure and valency ratio between Mn3+/Ru5+ and Mn4+/Ru4+. Reverse Monte Carlo simulations confirm that there is a shift in the B-site cation charge distribution from nearly equal amounts of Mn3+, Ru5+, Mn4+, and Ru4+ for SrMn0.5Ru0.5O3 to primarily Mn4+ and Ru4+ for CaMn0.5Ru0.5O3. The compounds Ba0.5La0.5Mn0.5Ru0.5O3, Ca0.5La0.5Mn0.5Ru0.5O3, and Sr0.5Ca0.25La0.25Mn0.5Ru0.5O3 were also investigated to study the effects of changing the charge of the A-site cation. Although substitution of La3+ for a divalent alkaline earth ion increases the Mn3+ content, this series of compounds also shows a relative increase in the concentration of Mn4+ as the average size of the A-site cation is decreased. In all compounds the octahedra containing Mn3+ are found to be Jahn-Teller distorted regardless of whether or not long range orbital ordering is observed, while the Ru-centered octahedra are symmetric. No evidence for short range cation ordering at either the A or B-sites was found for any of the compositions. This study also reports the previously undocumented finding that locally the A-site cations lie closer to the Mn ions than to the Ru ions and this asymmetry appears to be correlated to the degree of octahedral tilting.

Name	Saurabh Singh	LA-UR 12-20903
Group:	LANSCE-LC	
Mentor:	Jarek Majewski	
Field of Study:	Bioscience	
Discipline:	Biomedical Engineering	
Appointment:	Postdoc Research Associate	
Poster Title:	Swelling and Water Uptake of PEI/PSS Polyelectrolyte Multilayers	

ABSTRACT

We report here a structural investigation of polyelectrolyte multilayer films (PEMs) fabricated using layer-by-layer (LbL) self-assembly method. Ultrathin films prepared using a strong polycation, poly(ethylene imine) [PEI], and a strong polyanion, poly(styrene sulfonate) [PSS], were characterized using neutron reflectometry (NR). We also estimated the uptake of water and water vapors in PEM nanofilms.

Samples with 3 different layer thickness were prepared: (1) 5 layers [PEI/PSS]2-PEI, (2) 7 layers [PEI/PSS]3-PEI, and (3) 9 layers [PEI/PSS]4-PEI. NR data for the samples was collected in air, followed by which the measurements were performed in D2O saturated conditions. NR measurements were also performed for LbL films exposed to bulk D2O. It was found that the first few (i.e. 3 to 4) layers resulted in a noncontiguous or island type of deposition of polyelectrolytes, after which a more contiguous and uniform layer deposition began. Upon exposure to D2O saturated vapors, approximately 22%, 31%, and 45% swelling in the total film thickness were observed for 5, 7, and 9 layered PEMs samples, respectively. Nevertheless, no further increase in the film thickness was observed when the measurements were performed in bulk D2O. Roughness of 10 Å was estimated for all the samples measured in air. Moreover, no significant change in the PEMs roughness was observed when the measurements were performed in saturated D2O vapors and bulk D2O.

The amount of water uptake was characterized by swelling of the samples and the change in their water content – quantities which are independently accessible in a NR experiment. We understand that the practical application of PEMs requires full understanding of the role of main physiological factors affecting PEMS structure and interfacial behavior. We note that due to a broad range of polyelectrolytes which can be employed for a multilayer formation in various conditions, one has to restrict studies to characterize certain PEM system. Therefore, we limited this study to the understanding of PEMs formed from the interaction of strong polycation and polyanion (i.e. PEI and PSS).

Name	Claire White	LA-UR 11-03067
Groups:	LANSCE-LC and T-1	
Mentors:	Katharine Page and Neil Henson	
Field of Study:	Materials Science	
Discipline:	Combining Neutron Scattering and Computer Simulations	
Appointment:	Director's Postdoc Fellow	
Poster Title:	Multiscale Modeling of the Structure Mechanisms Occurring During the Formation of Geopolymer Binders: Combining Density Functional Theory and Monte Carlo Analysis	

ABSTRACT

'Geopolymer' concrete which is derived from coal fly ash and blast furnace slag activated by an alkali source has recently become an emerging area of research due to application as a sustainable alternative to traditional concrete (ordinary Portland cement-based concrete). The success of this material in the industrial setting is in large part due to the increasing pressure to use environmentally friendly materials, and with Portland cement accounting for 5-8% of global man-made CO2 emissions, geopolymer concrete is a viable alternative.

In order to attain a practical alkali-activated geopolymer concrete there has been extensive research into both the real-world material and a variety of associated model systems. In this paper, we outline how molecular research on these model systems using neutron and X-ray total scattering analysis and simulation techniques has contributed to understanding the structural mechanisms occurring during formation of the model systems. Techniques utilized include reciprocal-space and local structure analysis from total scattering, density functional modeling, and coarse-grained Monte Carlo simulations. Hence, by understanding the mechanisms responsible for the behavior of model systems, and therefore various aspects of the chemistry of the industrial counterpart especially at the nanoscale, there exists new evidence regarding the performance and durability of this new material.

LANSCE-NS

Name	Brent Perdue	LA-UR 12-00446
Group:	LANSCE-NS	
Mentors:	Robert Haight and Terry Taddeucci	
Field of Study:	Physics	
Discipline:	Nuclear and Neutron Science	
Appointment:	Postdoc Research Associate	
Poster Title:	Development of Neutron Detector Arrays for Neutron-Induced Reaction Measurements	

ABSTRACT

Development of arrays of detectors for the detection of neutrons and gamma rays produced in neutron-induced reactions at the Los Alamos Neutron Science Center (LANSCE) is ongoing, building on the solid foundation of past designs. Our current work is centered on the characterization of the types of neutron detectors that will be used in the arrays (liquid scintillators and 6Li-glass detectors) and the construction of the detector supporting structures. These arrays will be used to measure the outgoing neutron spectra in experiments at the Weapons Neutron Research (WNR) facility at LANSCE on neutron-induced fission and inelastic neutron scattering. These experiments will provide improved data for nuclear energy and security applications. Precise measurements of the outgoing neutron spectra following neutron-induced fission impact the areas of nuclear energy, criticality safety, and global security. Similar measurements of the outgoing neutron spectra from inelastic neutron scattering provide nuclear structure information, such as nuclear level densities in regions of high excitation energy. We outline tests and considerations toward understanding the important contributing factors to meeting our design goals.

Materials Physics and Applications Division
MPA-11

Name	John Brady	LA-UR 12-20958
Group:	MPA-11	
Mentors:	Dipen Sinha and Cristian Pantea	
Field of Study:	Physics	
Discipline:	Acoustics and Heat Transfer	
Appointment:	Postdoc Research Associate	
Poster Title:	Heating and Cooling with Sound Waves	

ABSTRACT

Under the right conditions, sound waves can be used to generate significant amounts of heating or cooling. At present, private industry—including the auto, oil, and computer industries—and the military are either researching or using this technology because it is inherently low-maintenance, environmentally friendly, and potentially cheaper than current alternatives.

One of the challenges in designing sound wave devices though, is that there is not much data available to predict their performance. By contrast, volumes of formulas are available to help predict heating or cooling generated by steady flows—such as wind blowing through a car radiator or a fan blowing on a heat sink, where air moves at a constant direction and speed. This leads to the question: can we use formulas developed for steady flows to predict the performance of sound wave devices? If so, the design process could become much simpler, thereby making the technology more market-ready.

This poster presents the results of a first-step study addressing this question.

Name	Anirban Chaudhuri	LA-UR 12-20799
Group:	MPA-11	
Mentor:	Dipen Sinha	
Field of Study:	Engineering	
Discipline:	Acoustics	
Appointment:	Postdoc Research Associate	
Poster Title:	Determination of Sound Speed and Composition in Oil-Water Mixtures using Non-Invasive Ultrasound	

ABSTRACT

Accurate measurement of the composition of binary fluid mixtures in real-time within the process environment is a challenging problem, particularly in the oil and gas extraction and petrochemical industries. Commercially available metering techniques are either off-line (manual sampling), invasive (density meters, capacitance probes), or expensive (microwave or gamma ray based schemes). The current work by the authors presents a method of accurately determining the volume fractions of two immiscible fluids in a two-phase flow by measuring the speed of sound through the composite fluid along with the instantaneous temperature. The use of externally mounted piezoelectric transducers allows the measurement to be non-invasive and offers considerable cost savings over currently available techniques. Sound speed in the composite medium is measured by transmitting a linear chirp signal and applying signal processing techniques. Two separate algorithms are developed to calculate volumetric composition, also known as "water-cut" in the oil industry, based on earlier work by Urick [Journal of Applied Physics, 1947] and Kuster & Toksoz [Geophysics, 1974]. The main difference between these two approaches is the representation of the composite density as a function of the individual densities; the former uses a linear rule-of-mixtures approach, while the latter uses a non-linear fractional formulation. The fluid densities and sound speeds are calibrated over the entire operating temperature regime for each fluid component, and the coefficients of the fitted polynomials are utilized in the final algorithm. Both methods lead to a quadratic equation with temperature-dependent coefficients, the root of which yields the volume fraction whose value lies between 0 and 1. We present results of studies with two different mixtures of crude oil and processed water, and also compare our results with a commercially available Coriolis density meter; the difference in mean values of water-cut computed by the two meters in long duration tests was less than 1%. Numerical studies of sensitivity of the calculated volume fraction to changes in temperature and sound speed are also presented; it is observed that the errors are lower if the two component fluids have more widely differing acoustic properties.

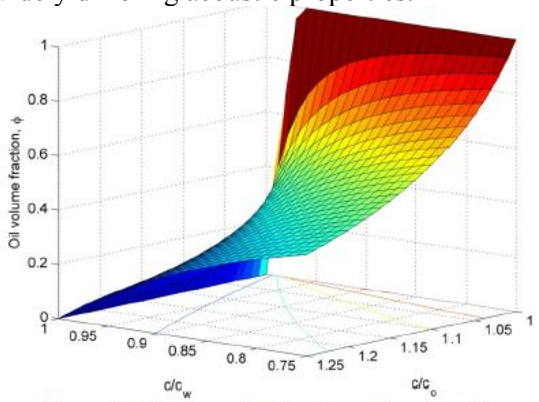


Figure 1: Oil volume fraction,ϕ, as a function of measured sound speed, c

Name	Qing Li	LA-UR 12-20894
Group:	MPA-11	
Mentor:	Piotr Zelenay	
Field of Study:	Materials Science	
Discipline:	Electrocatalysis and Fuel Cell	
Appointment:	Postdoc Research Associate	
Poster Title:	Anode Catalysts for the Direct Dimethyl Ether Fuel Cell	

ABSTRACT

While the direct methanol fuel cells (DMFC) is of particular significance for portable power sources, its performance is strictly limited by various factors, including the slow kinetics of methanol oxidation, crossover of methanol and ruthenium from the anode to the cathode side of the cell, and safety concerns about the methanol itself. Alternatively, dimethyl ether (DME), a widely used gas for aerosol propulsion, solvents and coolants, has been investigated in the last decade as a possible fuel for direct-feed fuel cells. When oxidized to CO2, one DME molecule releases 12 electrons in a reaction that does not require a C-C bond splitting. DME has higher energy density than methanol (8.2 vs. 6.1 kWh/kg). Due to a lower dipole moment, DME fuel crossover is generally less than that of methanol, with reduced impact on the cathode performance. DME is also less toxic than methanol, and can be conveniently stored and transported using existing infrastructure and storage technologies.

However, the DME electrooxidation at PtRu catalysts, remains kinetically handicapped relative to the oxidation of methanol. Therefore, developing a viable anode catalyst for DME oxidation is a key to improving the direct DME fuel cell (DDMEFC) performance. Taking the mechanism of DME electrooxidation on Pt into account, it seems that the activation barrier for the C-O bond cleavage may be responsible for the slower kinetics of DME oxidation compared to methanol. Since transition metals, such as palladium (Pd), are known to aid in the C-O bond splitting of ethers, an addition of Pd to the PtRu catalysts could also enhance catalytic activity in DME oxidation. Our preliminary half-cell measurements indicate that the specific activity of DME electro-oxidation measured with the homemade ternary Pt60Ru15Pd25/C (24% metal loading) catalyst is higher than that of a the-state-of-the-art Pt50Ru50/C catalyst for methanol oxidation (HiSPEC® 12100, 75% metal loading). Fuel cell polarization data further attest to the high activity of the PtRuPd/C anode in DME electrooxidation.

Name	Blake Sturtevant	LA-UR 12-20959
Group:	MPA-11	
Mentors:	Cristian Pantea and Dipen Sinha	
Field of Study:	Physics	
Discipline:	Acoustics	
Appointment:	Postdoc Research Associate	
Poster Title:	Sound Speed Measurements in Water up to 563 K and 11.7 MPa using a Novel and Rugged Sensor	

ABSTRACT

The speed of sound in a liquid varies with multiple physical properties including temperature, pressure, dissolved solid concentration and dissolved gas concentration. Sound speed measurements can thus be a powerful tool for characterizing geothermal and petroleum well downhole environments, particularly when used to complement existing temperature and pressure logging technologies. One challenge to making acoustics measurements in downhole environments is the design and construction of a rugged sensor that can withstand the extreme temperatures and pressures characteristic of these environments while still making high precision measurements. In this work, such a tool has been constructed and tested in a lab-based test environment designed to simulate geothermal well downhole pressures and temperatures. Two lithium niobate (LiNbO3) single crystal transducers were used to convert electrical energy into acoustic waves (and vice-versa) through the piezoelectric effect. Each of the transducers was packaged in a stainless steel housing constructed of off-the-shelf Conflat and Swagelok components. The two stainless steel packages were arranged such that the crystals were parallel and facing each other. In this configuration, one transducer acts as an acoustic transmitter while the other receives the acoustic signal. The test environment consisted of a high-pressure vessel (Parr Instrument Co.) rated up to 773 K and 24.5 MPa. Swept Frequency Acoustic Interferometry (SFAI), a LANL-developed technology, was used to measure sound speed. SFAI combines the frequencies of multiple acoustic resonant peaks with the distance between the transducers to determine the sound speed in a medium. The speed of sound in liquid water was measured in this work at ten pressures between ambient and 11.7 MPa along 18 isotherms between ambient and 563 K. These data represent the first direct measurements of water sound speed over this complete temperature and pressure range. The values reported here show very good agreement with water sound speeds listed in the International Association for the Properties of Water and Steam (IAWPS) tables, which have been derived from measurements of related thermodynamic quantities. The sound speed was found to increase from its room temperature value of 1482 m/s through a maximum of 1555 m/s near 348 K before monotonically decreasing to 990 m/s at 563 K. The pressure derivative of sound speed, dc/dP, which is directly related to the degree of non-linearity of a material, was found to vary strongly with temperature. Specifically, dc/dP increased by a factor of 5 from a value of 1.45 m/s/MPa at 293 K to 7.11 m/s/MPa at 538 K. This result demonstrates that, at high temperatures, non-linear effects become increasingly important.

Name	Blake Sturtevant (continued)	LA-UR 12-20959
Group:	MPA-11	
Mentors:	Cristian Pantea and Dipen Sinha	
Field of Study:	Physics	
Discipline:	Acoustics	
Appointment:	Postdoc Research Associate	
Poster Title:	Sound Speed Measurements in Water up to 563 K and 11.7 MPa using a Novel and Rugged Sensor	

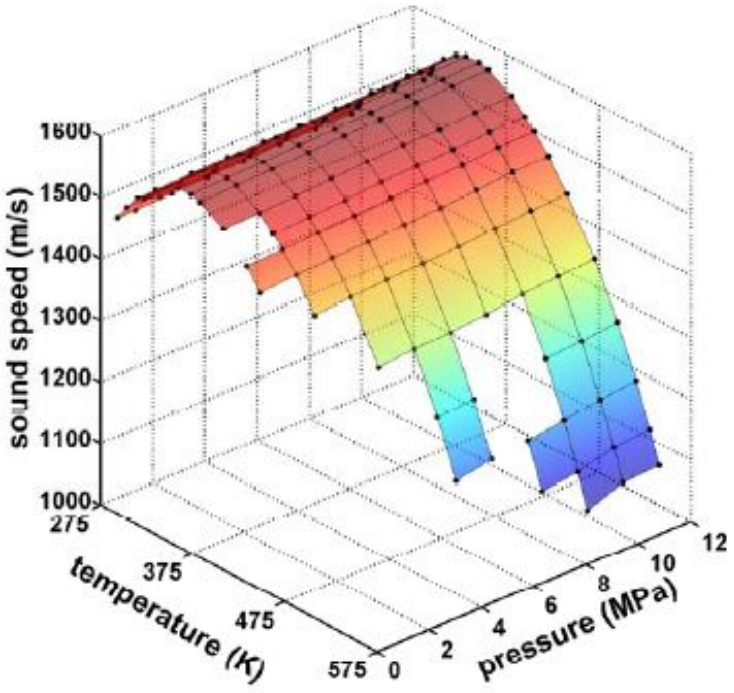


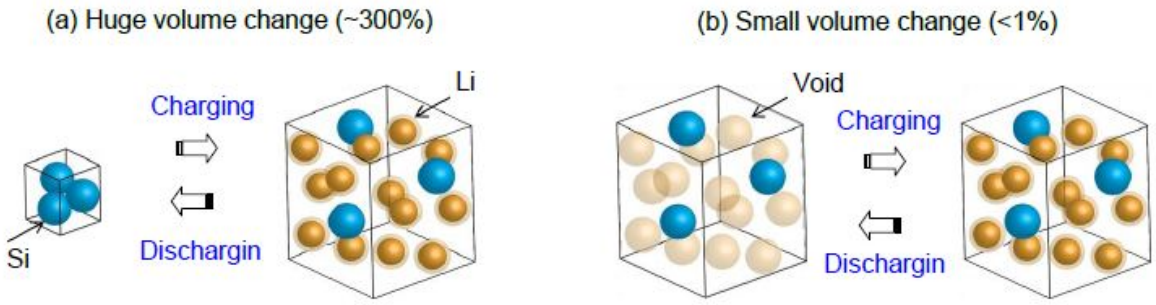
Figure: sound speeds in liquid water plotted as a function of temperature and pressure. The black circles represent measured data points.

MPA-CINT

Name	Jeong-Hyun Cho	LA-UR 12-20892
Group:	MPA-CINT	
Mentor:	Tom Picraux	
Field of Study:	Materials Science	
Discipline:	Energy Storage	
Appointment:	Postdoc Research Associate	
Poster Title:	Self-Optimization of Silicon Nanowires for Small Volume Change and a High Performance Lithium-Ion Battery Anode	

ABSTRACT

Lithium-ion batteries are widely used in portable electronic systems and electric vehicles because of their relatively high energy density, lack of a memory effect, and low self-discharge. However, the pace at which the energy capacity of batteries is improving is not fast enough to mitigate the energy consumption of new electronic systems. It is known that the energy capacity can be up to an order of magnitude larger than today's commercially available products by using silicon (Si) as an anode material. However, the mechanical stress due to silicon's volume change (approximately 300%) during charging and discharging (the insertion and extraction of Li ions, Fig. a) quickly destroys the electrode and leads to the loss of electrical contact between the anode material (Si) and a current collector. In order to alleviate the pulverization of the anode material, a self-assembly (self-optimization) process is developed to reduce the volume change of Si from 300% to less than 1% during cycling without sacrificing high specific capacity. The self-optimization process generates internal voids within Si for Li-ion occupation with minimum volume change (Fig. b) and realizes significantly improved long-term cyclability.



Name	Wei Gao	LA-UR 12-20899
Group:	MPA-CINT	
Mentors:	Andrew Dattelbaum and Aditya Mohite	
Field of Study:	Chemistry	
Discipline:	Chemistry	
Appointment:	Director's Postdoc Fellow	
Poster Title:	Direct Laser Writing of Micro-Supercapacitors on Hydrated Graphite Oxide Films	

ABSTRACT

Microscale supercapacitors provide an important complement to batteries in a variety of applications, including portable electronics. Although they can be manufactured using a number of printing and lithography techniques, continued improvements in cost, scalability and form factor are required to realize their full potential. Here, we demonstrate the scalable fabrication of a new type of all-carbon, monolithic supercapacitor by laser reduction and patterning of graphite oxide films. We pattern both in-plane and conventional electrodes consisting of reduced graphite oxide with micrometre resolution, between which graphite oxide serves as a solid electrolyte. The substantial amounts of trapped water in the graphite oxide makes it simultaneously a good ionic conductor and an electrical insulator, allowing it to serve as both an electrolyte and an electrode separator with ion transport characteristics similar to that observed for Nafion membranes. The resulting micro-supercapacitor devices show good cyclic stability, and energy storage capacities comparable to existing thinfilm supercapacitors.

Name	Nathaniel Grady	LA-UR 12-20991
Group:	MPA-CINT	
Mentor:	Hou-Tong Chen	
Field of Study:	Materials Science	
Discipline:	Nonlinear Optics	
Appointment:	Postdoc Research Associate	
Poster Title:	Nonlinear Terahertz Response of High-Temperature Superconducting Films and Metamaterials	

ABSTRACT

Metamaterials consisting of arrays of conducting elements are a powerful tool for controlling electromagnetic energy in frequency ranges where natural materials are limited (e.g. THz) and to create materials exhibiting exotic electromagnetic phenomena not observed in natural materials (e.g. negative refraction). While metals have been used for the conductive elements in the vast majority of metamaterial structures, the use of superconductors is of rapidly growing interest due to their superior conductivity at low temperatures, their intrinsic magnetic field and temperature dependent complex conductivity which is naturally suited for creating active metamaterial devices, and the potential to integrate elements exhibiting quantum behavior.

Recently developed high power THz sources based on tilted-pulse-front optical rectification are opening up new windows into the nonlinear response of materials in the THz frequency range. We report the observation of a nonlinear THz response of high-temperature superconducting films and split ring resonator arrays made of high-temperature superconducting films. Intensity-dependent transmission measurements indicate a suppression of superconductivity at high intensities. For metamaterials, this results in the resonance strength decreasing dramatically (i.e. transient bleaching) and the resonance frequency shifting as the intensity is increased. Pump-probe measurements confirm this behavior and reveal dynamics on the picosecond time scale.

In conclusion, we have observed strong nonlinearities in the THz response of high-Tc superconducting films and metamaterials. These observations are not only of practical interest for developing active and nonlinear metamaterial devices, but also of fundamental interest due to their potential to improve our understanding of the physics of high-Tc superconductivity.

Name	Yoontae Hwang and Jennie Schei	LA-UR 12-20902
Groups:	MPA-CINT and P-21	
Mentors:	Shadi Dayeh, Tom Picraux, and John George	
Field of Study:	Materials Science	
Discipline:	Device Fabrication and Characterization	
Appointment:	Postdoc Research Associate	
Poster Title:	High-Density Capacitive Pillar Arrays for High Fidelity Neural Sensors	

ABSTRACT

Sensing neural activity from an individual neuron cell is essential to decrypt signal transport and processing in functional neural networks. If achieved, such high spatial resolution would allow fulfilling long-term sought objectives in neuroscience and neuroprosthetics: understanding the biological basis for our consciousness, and controlling artificial limbs for injured people, respectively. This requires developing compact, highly sensitive, high-resolution and high-density, implantable 3D probes that are well beyond current microprobe techniques. Current neural electrodes operate by a direct charge interaction between ions in the cellular medium and charge carriers in the electrodes through redox reactions, which can cause a significant damage to the cell as well as a degradation of the electrodes. Here, we present a novel capacitive neural-sensing technique that bypasses direct charge interaction between the electrode arrays and neuron cells, and enables sub-cellular neural activity detection with potential for high-fidelity electro-neural interfaces.

Figure 1 shows a schematic cartoon of our targeted neural sensing platform. In order to achieve individual addressability in our high-density electrodes, the Si-based nano-pillar arrays need to be integrated on insulating substrates such as sapphire. However, due to the lattice mismatch between Si and sapphire, growth of silicon on sapphire substrates is not possible without severe defects that will limit the performance of our devices. We invented a novel all-solid state wafer bonding technique that allowed integration of our nano-pillar arrays to patterned (electrically isolated) electrode leads on sapphire substrates. Silicon wafers (p-type, 50 μm) were bonded to sapphire by a controlled silicidation process and were then thinned down to 10 μm, which is the desired length of our nano-pillar arrays. A combination of photolithography and e-beam lithography then followed to pattern nickel (100 nm) dots as masks for inductive coupled plasma (ICP) etching of our high aspect ratio Si pillars. To achieve capacitive sensing mechanism, we developed a process for the epitaxial growth of thin n-doped shells over our ntype pillars to create a totally depleted p-n junction at the surface of our nano-pillar, which is then followed by high dielectric constant oxide deposition (HfO2 by atomic layer deposition) for high capacitance sensitivity and for bio-compatibility.

These devices will allow safe, lower power, corrosion resistant and high resolution probes not only for in-vitro but also for in-vivo physiological experiments. Preliminary physiological sensing experiments will be presented.

Name	Yoontae Hwang and Jennie Schei (continued)	LA-UR 12-20902
Groups:	MPA-CINT and P-21	
Mentors:	Shadi Dayeh,Tom Picraux, and John George	
Field of Study:	Materials Science	
Discipline:	Device Fabrication and Characterization	
Appointment:	Postdoc Research Associate	
Poster Title:	High-Density Capacitive Pillar Arrays for High Fidelity Neural Sensors	

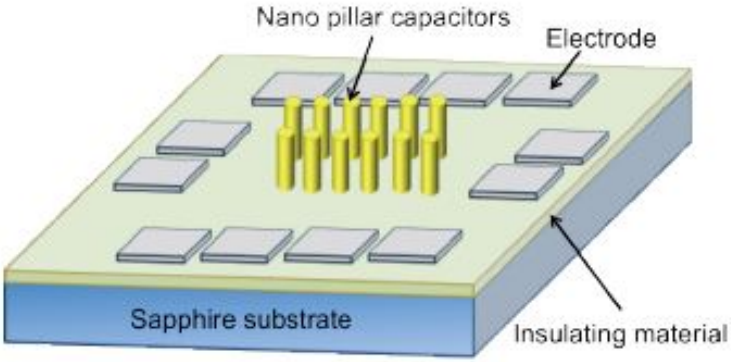


Fig. 1: Schematic image of nanopillar capacitor arrays for single neuron detection. Each nanopillar is connected to each electrode under insulating material. Thus, each nanopillar is perfectly electronically-isolated to each other.

Name	Binh-Minh Nguyen	LA-UR 12-20887
Group:	MPA-CINT	
Mentors:	Shadi Dayeh and Tom Picraux	
Field of Study:	Engineering	
Discipline:	Electrical Engineering	
Appointment:	Director's Postdoc Fellow	
Poster Title:	One Dimensional Transport in Ge/Si Core/Shell Nanowires: Physics and Device Applications	

ABSTRACT

Transport in one-dimensional semiconductor structures possesses unique properties, which attract great attention for both basic research and device applications. For example, in 1D nanowire structures where the charge carrier transport length is comparable to their mean free path, carriers are free from elastic and inelastic scattering, and can travel ballistically. As a result, the wire resistance remains constant, regardless of its length. This contradiction to the conventional Ohm's law triggers interests in exploring fundamental physics of 1D ballistic effects, as well as prompts novel device concepts using this high-speed transport. However, observing ballistic transport and making use of it are normally obstructed by the difficulties achieving high material quality and minimizing detrimental perturbations from surface processes.

In this work, Ge/Si concentric nanowire materials are utilized as a platform for studying hole ballistic transport in 1D semiconductor channels and to demonstrate ballistic and high performance field effect transistors (FETs). The nanowire structure consists of a Ge core and a higher band gap Si shell in order to spatially confine holes inside the core of the nanowire, thus minimizing surface scattering and surface trapping effects. Advanced material growth of Ge/Si core/shell nanowires with abrupt doping and composition interfaces were achieved with chemical vapor deposition allowing for high quality materials with long carrier mean free path, to the extent that it can be observable, and deployable in electronic devices. As grown wires were then coated with high-k HfO_2 gate dielectric and transferred on a SiN template for fabrication of single nanowire devices. Scanning electron microscopy was utilized to record wire coordinates and e-beam lithography was used to write masks for subsequent processing steps. Window opening through the HfO_2 layer was performed with wet chemical etching prior to nickel electrode deposition. Sub-100 nm ultra-short channels were further achieved by a controlled germanidation/silicidation reaction of nickel electrodes at elevated temperatures. Finally, titanium/gold gate contacts were deposited precisely on top of the ultra-short unsilicided channel. Room temperature transport characterization and analysis was then performed. Preliminary results show that these Ge/Si heterostructure FETs exhibit high on/off current ratios up to 10^5 and sub-threshold swings of 180 mV/decade with on-current performance of 6 μA at 100mV V_{DS}, which is expected to exceed state of the art with further device optimization.

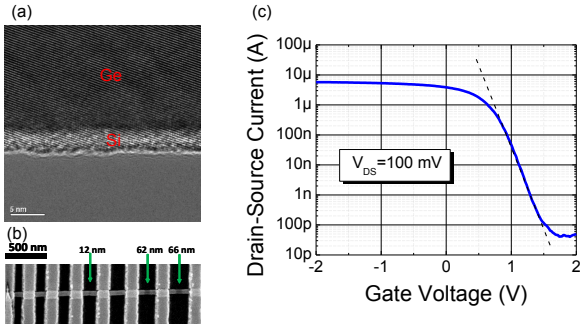


Figure: (a) high resolution TEM image showing high quality Ge/Si core/shell structure. (b) SEM image of a processed single wire device with ultra-short channel (~12nm), (c) Id-Vg characteristics of a Ge/Si FET.

Name	Douglas Shepherd	LA-UR 12-20672
Groups:	MPA-CINT, CCS-3, and T-CNLS	
Mentors:	James Werner and Brian Munsky	
Field of Study:	Bioscience	
Discipline:	Single Molecule Biophysics	
Appointment:	Postdoc Research Associate	
Poster Title:	Spatio-Temporal Measurements and Modeling of Genetic Expression	

ABSTRACT

Single-molecule, single-cell studies of genetic expression have provided key insights into how cells respond to external stimuli [1-5]. By directly measuring copy numbers of individual biomolecules in cells, such as the number of individual messenger RNA transcripts, it is now possible to obtain statistical measures of the spatio-temporal distributions of key signaling and regulatory molecules. Such comprehensive datasets can be used to infer system-level models that yield quantitative insight into cellular regulation, predict cellular responses in new experimental conditions, and suggest more revealing experiments to uncover regulatory dynamics. The integration of single-molecule spectroscopy, biochemistry, and numerical modeling is a powerful multi-disciplinary approach to investigating cellular response at the genetic level.

We have constructed a microscope and data analysis package capable of automated, multiplexed measurements of mRNA transcripts fluorescently tagged via smFISH [5,6]. This capability enables visualizing the spatial distribution of single mRNA transcripts in large populations of single cells and builds rich datasets for gene expression pathways. In turn, these data sets allow quantitative explorations of spatio-temporal fluctuations of mRNA within cells. A key issue we seek to address is what types of fluctuations are most informative about the underlying gene regulatory process. In other words, how much experimental resources should be spent to measure (i) temporal, (ii) spatial, or (iii) cell-to-cell fluctuations? As an example, we studied Interluekin 1-alpha (IL1α) mRNA expression within human THP-1 cells during stimulus response to lipopolysaccharide (LPS). By spatially resolving mRNA within thousands of individual cells and at multiple times points, we quantified all three fluctuation types [6].
We then expanded the common bursting gene expression model [7] and derived a set of linear ODEs to describe the mean, variance, and co-variance of nuclear and cytoplasmic IL1α mRNA. We fit this model to the full single-cell data set from above. Next, we used this baseline model to simulate limited data sets that contain different combinations of the three fluctuation types. Comparing models inferred from each simulated data set, we are able to draw conclusions on which fluctuation types are most revealing about the underlying system's mechanisms and parameters. Using the results of this computational investigation, we are able to design the next round of experiments to provide maximal discrimination power between competing archetypes of IL1α mRNA production and regulation.

The approach developed here is applicable to any eukaryotic gene expression pathway. With careful integration of discrete spatial stochastic analyses and single-molecule experimental measurements of mRNA expression, one can design more informative experiments, capture spatial, temporal and cell-to-cell fluctuations, and uncover new insight into gene regulatory phenomena.

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Name	Jinkyoung Yoo	LA-UR 12-20886
Group:	MPA-CINT	
Mentor:	Tom Picraux	
Field of Study:	Materials Science	
Discipline:	Semiconductor and Nanotechnology	
Appointment:	Postdoc Research Associate	
Poster Title:	Single Crystalline Si Radial p-i-n Nanowire Arrays for Photovoltaic Applications	

ABSTRACT

Si radial p-n junction nanowires (NWs) provide new opportunities as photovoltaic (PV) components with high photoconversion efficiency due to orthogonalization of light absorption direction and carrier separation directions. However realization of high-performance Si radial NW photovoltaic cells and elucidation of their carrier transport has been demanding. Previous methods of forming radial p-n junctions have emphasized Si NW growth followed by diffusion doping or amorphous Si layer deposition, limiting the tuning of the p-n junction interfaces and achievement of high photovoltaic device performance. Here we present excellent quantum efficiency of single crystalline Si radial p-i-n junction arrays prepared by controlled low temperature homoepitaxial growth of single crystalline Si radial shells. Single crystalline Si radial p-n junctions consisted of core p-type Si NWs and n-type Si shells. Dimensions and electrical doping profiles of core Si NWs and epitaxial Si shells were precisely controlled by e-beam lithography and Si deep reactive ion etching followed by low-pressure chemical vapor deposition growth. Vertical NW array with pitch in the range of 1 to 2 micrometers were studied and the diameters and lengths were varied from 100 to 700 nm and 5 to 10 micrometers, respectively.

The radial undoped and doped n-type Si shells were grown epitaxially on the surfaces of Si nanowires in the range of 670 to 810^{o}C by chemical vapor deposition. In the nanoscale radial growth process we found single crystalline shell growth with a progressive increase in surface roughness and then a breakdown in single crystal epitaxy followed by rapid polycrystalline shell growth at a critical thickness. The critical thickness increases with increasing temperature such that well-faceted and fully crystalline shells in the 100's of nanometer range are obtained at the higher temperatures. Using these processes vertical single crystalline Si radial p-n junction NW arrays and single NWs structures were grown and their optical, electrical and PV response were characterized. We separate the contributions of enhanced optical absorption due to the NW light scattering and the carrier separation in the radial Si p-n junctions to the PV response as a function of NW spacing and length. Finally we observed the best reported quantum efficiency of radial p-n junction PV cells.

Name	Shixiong Zhang	LA-UR 12-20889
Group:	MPA-CINT	
Mentor:	Tom Picraux	
Field of Study:	Materials Science	
Discipline:	Materials Physics and Nanoscience	
Appointment:	Director's Postdoc Fellow	
Poster Title:	Synthesis, Characterization and Magneto-transport Studies of a New Generation of Electronic Materials: 3-D Topological Insulators	

ABSTRACT

Recently a new class of electronic materials, called topological insulators, has been discovered. They are different from previous materials in that they are characterized by the topologically protected metallic surface states, which coexist with their insulating bulk states. The unique surface states consist of a single Dirac cone and the resulting Dirac Fermions on the surface are robust against any nonmagnetic impurities or disorder as a result of strong spin-orbit coupling and time-reversal symmetry. Such topological insulators are predicted to exhibit a number of striking electromagnetic properties and may offer new applications in spintronics and quantum computations. Here, we report our magneto-transport studies on a number of topological insulators in both thin film and nanowire forms to reveal the topological surface properties. The TI thin films were epitaxially grown by pulsed laser deposition and single crystalline nanowires were synthesized by thermal vapor deposition. In particular, we observed a two dimensional weak anti-localization effect in thin films at low temperatures, which reflects the destructive quantum interference between the Dirac fermions travelling along two time-reversed self-crossing loops. More importantly, we observed linear magnetoresistance (MR) as the magnetic field (from a few Tesla up to 60 Tesla) was applied perpendicular to the surface of the films and nanowires. This linear MR is believed to be associated with the quantization of the surface Dirac Fermions that all occupy the lowest Landau levels under the influence of strong magnetic fields.

MPA-CMMS

Name	Oscar Ayala-Valenzuela	LA-UR 12-20999
Group:	MPA-CMMS	
Mentor:	Ross McDonald	
Field of Study:	Physics	
Discipline:	High Magnetic Fields	
Appointment:	Postdoc Research Associate	
Poster Title:	Challenges at 100T Science	

ABSTRACT

The recently achieved 100T multi-shot world record by The National High Magnetic Field Laboratory in Los Alamos has been a result of the workforce of numerous talented people, besides this goal, six different experiments have been carried out during the same magnetic pulse (e.g. Eun D. Mun's poster) thanks to State of the Art Instrumentation techniques measuring selected samples; among them, High Temperature Superconductors, Molecular Magnets and Spin Frustrated Materials. Induction techniques present susceptibility to electromagnetic noise, which is always present in the system, High Frequency techniques are more desirable because of the magnetic pulse duration and dB/dt effects, optics techniques have been shown excellent and clean results. More theoretical work is needed to understand magnetic measurements and effects detected in novel materials, i.e. Topological Insulators, Nanomaterials and new superconductors, among others. This unique capability in the world has proved to be ready to face the new challenges in Physics and Materials Science at 100 T and beyond.

Name	Ryan Baumbach	LA-UR 12-01046
Group:	MPA-CMMS	
Mentor:	Eric Bauer	
Field of Study:	Physics	
Discipline:	Correlated Electron Physics	
Appointment:	Director's Postdoc Fellow	
Poster Title:	Search for Quantum Criticality in CeRu2M2X (M = Al and Ga, X = B and C)	

ABSTRACT

During the past several decades, research on systems that include transition metal, lanthanide, and actinide elements has led to a point of view that is summarized by the Doniach phase diagram, where the tendency of d or f electrons to localize or delocalize is driven by a competition between the RKKY and Kondo interactions [1]. In this picture, the competition between these two interactions can suppress a magnetic phase transition to absolute zero temperature, resulting in a quantum phase transition, around which new and distinct states (e.g., non-Fermi-liquid behavior and unconventional superconductivity) are often found which do not conform to the standard model of the metallic state (e.g., Fermi liquid theory) [2]. In conjunction with these issues, certain types of crystal structures have proven to be common themes (e.g., ThCr2Si2 and HoCoGa5-type), suggesting that the details of the d- or f-electron element environment play a significant role in how the physical state emerges. For these reasons, we were motivated to search for 4f-electron variants of the newly discovered LaRu2Al2B [3], which forms in a stuffed version of CeMg2Si2 and can be viewed as an alternative stacking arrangement of ThCr2Si2. This effort produced CeRu2Al2B, which exhibits localized 4f magnetic ordering at high temperatures; antiferromagnetism develops below a Néel temperature TN = 14.2 K and a first order ferromagnetic transition is observed at a Curie temperature TC = 12.8 K. The application of a magnetic field results in a rich T-H phase diagram [4]. Motivated by this discovery, we searched for other variants wherein chemical pressure might induce hybridization. During this search, we have identified CeRu2Ga2B and CeRu2Ga2C, both of which have smaller unit cell volumes than CeRu2Ga2B but still exhibit local moment ferromagnetism at temperatures TC = 16.3 K and 17.1 K, respectively. On a parallel track, we explored the influence of applied pressure on these compounds. In this seminar, I will give a summary of our results and discuss prospects for driving these compounds towards stronger hybridization. In particular, this effort is of interest because materials that are suitable for studying ferromagnetic quantum phase transitions are uncommon, although still of fundamental importance in understanding the quantum criticality conundrum, as recently pointed out by the theoretical work of Yamamoto and Si [5].

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[2] H. v. Löhneysen, et al., Rev Mod Phys 79, 1015 (2007)
[3] J. V. Zaikina, et al., Inorg. Chem. 49, 2773 (2010)
[4] R. E. Baumbach, et al., Submitted to Phys. Rev. B (2012)
[5] S. J. Yamamoto and Q. Si, Proc. Natl. Acad. Sci. 107, 15704 (2010)

Name Miles Beaux
Group: MPA-CMMS
Mentor: John Joyce
Field of Study: Physics
Discipline: Photoemission Spectroscopy
Appointment: Postdoc Research Associate
LA-UR 12-20893
Poster Title: Electronic Structure of Polycrystalline δ-Pu Metal: A Review of Photoemission Spectra Interpretations

ABSTRACT

We exploit our capability for photoemission spectroscopy (PES) measurements of Pu materials to present a systematic study of polycrystalline δ-Pu metal. Laser ablation was used to clean the surface of Ga stabilized δ-Pu and cleanliness was monitored through O 1s and Pu 4f core levels, as well as valence band features. Observation of these spectra provides better insight into the differentiation of contaminant features versus the strong correlation effects within Pu metal. Comparison to the Pu chalcogenide PuTe is used to better understand the origin of the three-peak structure observed in the valence band regions of both these and other Pu materials. Previously published interpretations of this three-peak structure are discussed relative to experimental spectral data. Subtraction of this three-peak structure from the valence band spectrum of δ-Pu is attempted in order to produce a better representation of electronic structure and compared to theory.

Name	Yan Li	LA-UR 12-20998
Groups:	MPA-CMMS and T-4	
Mentors:	Scott Crooker and Darryl Smith	
Field of Study:	Physics	
Discipline:	Condensed Matter Physics	
Appointment:	Director's Postdoc Fellow	
Poster Title:	Revealing Spin Dynamic Properties of Holes in Quantum Dots by "Listening" to Intrinsic Spin Noise	

ABSTRACT

Single electrons or holes (absence of an electron) confined in semiconductor quantum dots are one of the leading candidates for solid-state quantum bit, as the spin up or down is a natural way of representing "0" or "1" for quantum information storage and processing. One basic requirement for quantum bit is that the spin lifetime is long enough to perform all the computations before the carried information is lost. We study spin dynamic properties of single holes in (In,Ga)As quantum dots by passively "listening" to the intrinsic fluctuations of spins --- the spin noise. The measurement is perturbation-free magnetic resonance in the frequency domain, which tells us useful information about spin lifetimes and how exactly the spin decays. We observed clear evidence of hole spin relaxation by hyperfine interactions with the nuclei. The spin lifetimes are considerably long at zero magnetic field and it increases by one order of magnitude in a small longitudinal magnetic field to 5 micro seconds. Furthermore, the functional form of spin decay changes with the application of longitudinal field, as some spin relaxation channels are turned off.

Name	Eundeok Mun	LA-UR 12-20940
Group:	MPA-CMMS	
Mentor:	Vivien Zapf	
Field of Study:	Physics	
Discipline:	High Magnetic Field Science	
Appointment:	Postdoc Research Associate	
Poster Title:	Magnets and Science at the NHMFL	

ABSTRACT

Recently, a 100 T magnetic field which is the highest non-destructive magnetic field in the world was created by researchers at the National High Magnetic Field Laboratory (NHMFL) at Los Alamos National Laboratory. The purpose of pulsed magnetic field facility is not to achieve the highest magnetic fields, but to create the best research environment and to provide users. The user program is designed to provide researchers with a balance of the highest research magnetic fields and robust scientific diagnostics.

In this poster presentation, the pulsed magnetic field facility will be introduced. A pulsed magnet is designed to produce magnetic fields that are so large that the magnet cannot be energized for more than a very short period of time without destroying itself. The magnet is hooked up to an energy storage device, either a capacitor bank or a generator, and all the energy is dumped into the magnet in the course of a short period of time, from microseconds through milliseconds to a fraction of a second. The study of physics phenomena at the extreme conditions of temperature, pressure, and magnetic fields is a vital component at NHMFL's research aimed at understanding the physics of structurally complex systems at a quantum level. As examples of pulsed magnetic field research, the experimental results of the magnetoelectric effect in quantum magnet and high temperature superconductor will be presented.

Name	Benjamin Ueland	LA-UR 12-20860
Group:	MPA-CMMS	
Mentor:	Joe Thompson	
Field of Study:	Physics	
Discipline:	Magnetically Frustrated Strongly Correlated Electron Materials	
Appointment:	Postdoc Research Associate	
Poster Title:	Controllable Geometrical Hall Effect in a Frustrated Highly-Correlated Metal	

ABSTRACT

A current of electrons traversing a landscape of localized spins possessing non-coplanar magnetic order gains a geometrical (Berry) phase, which can lead to a Hall voltage independent of the spin-orbit coupling within the material--a geometrical Hall effect. We show that the highly correlated metal UCu5 possesses an unusually large controllable geometrical Hall effect at T<1.2K due to its frustration-induced magnetic order. The magnitude of the Hall response approaches 10% of the v=1 quantum Hall effect per atomic layer, which translates into an effective magnetic field of H~102T acting on the electrons. The existence of such a large geometric Hall response in UCu5 opens a new field of inquiry into the importance of the role of frustration in highly correlated electron materials.

Name	Franziska Weickert	LA-UR 12-21085
Group:	MPA-CMMS	
Mentor(s):	Roman Movshovich and Filip Ronning	
Field of Study:	Physics	
Discipline:	Condensed Matter Physics	
Appointment:	Director's Postdoc Fellow	
Poster Title:	Comparative Study of the Low-Temperature Thermodynamic Properties at the Field-Induced Quantum Critical Points in Pure and Br-Doped $NiCI_2$-4SC$(NH_2)_2$	

ABSTRACT

$NiCl_2$-4SC$(NH_2)_2$ (DTN) is an insulating magnetic material with a quantum paramagnetic ground state, which shows field induced XY antiferromagnetic (AFM) order between Hc1 = 2.1 T and Hc2 = 12.6 T at low temperatures. In boson language, the ground state of DTN can be described as a Mott insulator, and the ordered state as a Bose-Einstein condensation (BEC) of magnons. Bond disorder is introduced to the system by substituting Br atoms on Cl positions that simultaneously change the super exchange interaction along the c-direction on a local scale and lead to a Mott-glass ground state in zero field. For magnetic fields $0 < H < Hc1$ and $H > Hc2$, Br doped DTN develops a gapless Bose glass behavior, followed by a Mott insulating state above the saturation field Hsat. The critical fields Hc1,2 of the AFM order and the saturation field Hsat are shifted slightly by 8 % doping compared to those of pure DTN.

In the poster, we present a comprehensive experimental study of the low-temperature thermodynamic properties at the quantum critical points (QCPs) occurring at Hc1 in single crystals of pure and doped DTN, respectively. We find that the specific heat, magnetization, thermal expansion and the Grüneisen parameters in pure DTN can be well described by a BEC QCP with effective dimensionality $D = 3 + z = 5$. In contrast, the specific heat and magnetization data observed at Hc1 in Br-doped DTN obey temperature power laws with completely different exponents indicating the existence of a new, so-called Bose-glass QCP.

Our experimental results are supported by detailed and extensive analytical calculations quantum Monte-Carlo simulations of both systems.

Name	Marcus Weigand	LA-UR 12-20927
Group:	MPA-CMMS	
Mentor(s):	Boris Maiorov and Leonardo Civale	
Field of Study:	Physics	
Discipline:	Condensed Matter Physics	
Appointment:	Postdoc Research Associate	
Poster Title:	Alternative Routes to Enhance the Performance of Superconductors	

ABSTRACT

Due to their unique property of zero electrical resistance, superconductors lend themselves to a multitude of applications that require the ability of passing large electrical currents with low or no dissipation. Magnetic fields, which are present in most of these scenarios, penetrate a superconductor in the form of magnetic flux lines or vortices. Any applied current exerts a force on them, which leads to vortex movement and consequently energy dissipation once a certain critical current is exceeded. This problem can be tackled (i) by enhancing the pinning forces that hold flux lines in place and (ii) by reducing the dissipation once they start moving. The standard method for (i) is to generate a zone where superconductivity is suppressed that acts as pinning center for vortices. This approach has been 'exhausted', and there is a need for novel/alternative methods to achieve (i) and (ii). Theoretical work predicts that magnetic inclusions or layers can achieve both of these goals [1, 2].

In order to exploit these phenomena for future applications, however, a better understanding is required of the mechanisms that govern the interaction between superconducting vortices and magnetic media. We have focused on the family of borocarbides (RENi2B2C, where RE = rare earth) [3]. These materials exhibit both superconductivity and antiferromagnetism, thus representing an ideal 'toy box' to study above-mentioned effects.

We have conducted transport current-voltage and magnetization measurements on ErNi2B2C single crystals. In excellent agreement with each other, these experiments show a significant enhancement of the critical current at the Néel temperature (at which the material becomes antiferromagnetic). We analyze this increase in critical current as a result of the creation of antiphase boundaries at the antiferromagnetic transition.

[1] L.N. Bulaevskii, E.M. Chudnovsky, and M.P. Maley, Appl. Phys. Lett. 76, 18, 2594 (2000)
[2] A. Shekhter, L.N. Bulaevskii, and C.D. Batista, Phys. Rev. Lett. 106, 037001 (2011)
[3] P.C. Canfield, P.L. Gammel, and D.J. Bishop, Phys. Today 51, 10, 40 (1998)

MPA-MC

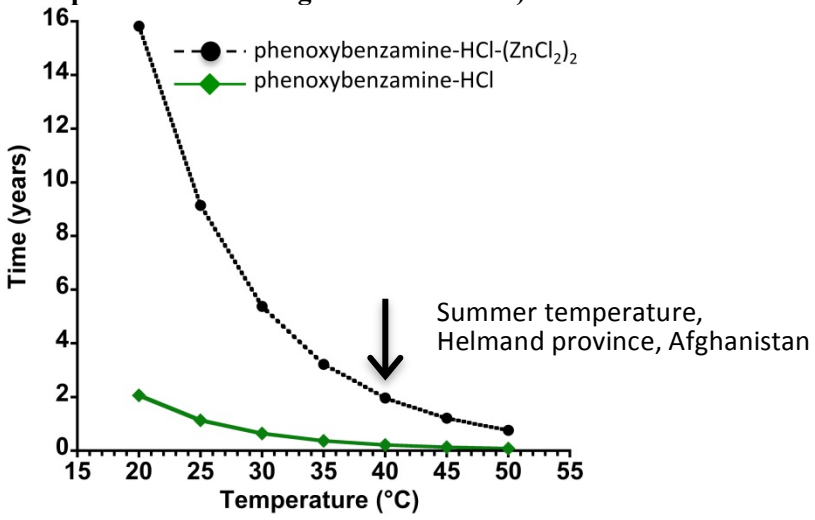
Name	Katherine Lovejoy	LA-UR 12-20821
Group:	MPA-MC	
Mentor:	Rico Del Sesto	
Field of Study:	Chemistry	
Discipline:	Bioinorganic	
Appointment:	Distinguished Reines Postdoc Fellow	
Poster Title:	Bioinorganic Ionic Liquid Formulations of Pharmaceuticals for Stability and Anti-Pathogen Activity	

ABSTRACT

We demonstrate a broadly applicable approach to the formulation of cationic pharmaceuticals that involves their conversion to amorphous ionic liquids using generally recognized as safe metal chlorides. Ionic liquid forms of active pharmaceutical agents address several critical medical needs of the warfighter. The pairing of cations and anions, at least one of which is an active pharmaceutical agent, to produce an amorphous molten salt that melts near room temperature generally improves shelf life, solubility, and bioavailability, and circumvents issues related to crystal polymorphism. The use of FDA-approved reagents in the formulations will facilitate translation to field use. The strategy is generally applicable to any pharmaceutical agent that can be generated as a chloride salt with a melting point lower than about 300°C. We present materials with potent anti-biofilm activity against antibiotic-resistant *Pseudomonas aeurginosa* biofilms.

Combination of a metal chloride and an organic chloride salt produces chlorometallate ionic liquids. Amorphous phases tend to be favored over crystallization if several anions exist in dynamic equilibria. The optimal stoichiometry for ionic liquid formation with zinc chloride is a 2:1 ratio of $ZnCl_2$-to-organic chloride salt ratio. The excess chloride forces an amorphous zinc melt by allowing formation of multiple fluidizing chlorozincate species including $[Zn_3Cl_8]^{2-}$ and $[Zn_4Cl_{10}]^{2-}$ which we observe by Raman spectroscopy and other methods.

Shelf Life (5% Decomposition of Starting Pharmaceutical)



Name	Biswajit Paik	LA-UR 12-10494
Group:	MPA-MC	
Mentor:	Troy Semelsberger	
Field of Study:	Materials Science	
Discipline:	Materials Chemistry	
Appointment:	Postdoc Research Associate	
Poster Title:	Ammonia Borane in Ionic Liquid: A Future Automotive Fuel?	

ABSTRACT

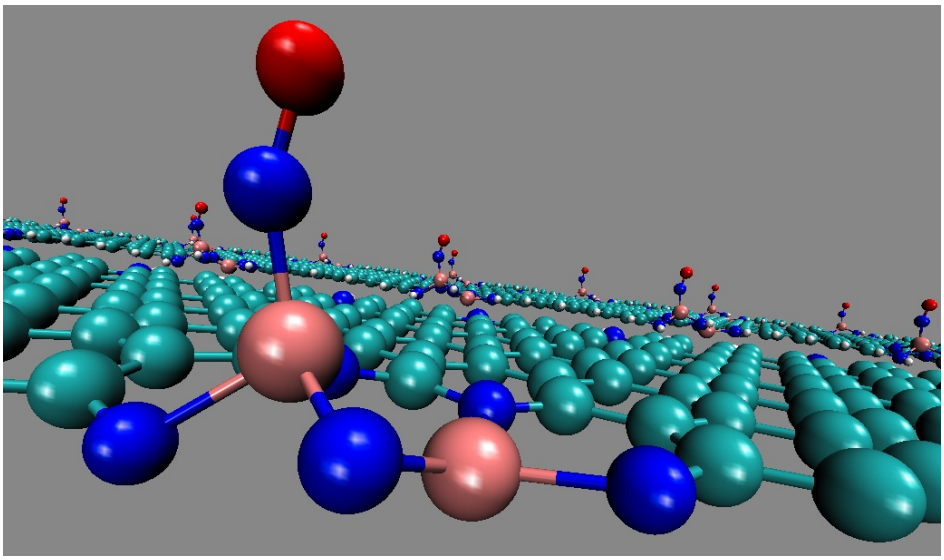
In the backdrop of grim energy and environmental situation on the global scale, hydrogen based energy infrastructure appears to be one of the viable options, especially, for automobile industry where the focus of state-of-the-art research is developing a reversible hydrogen (H_2) storage system with more than 5.5wt% storage capacity, as recommended by department of Energy (DOE), USA, for a system capable of operating onboard within the fuel cell temperature. A high hydrogen storage capacity of 19.6 wt% in ammonia borane (NH_3BH_3, or AB) motivates our research program to utilize the full potential of this hydride as a future automotive fuel. It is known that the solid AB releases more than 2/3 of its total hydrogen content within 150 °C during the thermal decomposition; the downside includes the uncontrollably fast reaction and the byproducts of the reactions in the form of ammonia, borazine, and diboarne which are not suitable to the usual fuel cell operation. In order to establish a control over the reaction kinetics and minimizing the amount of the undesired byproducts, ionic liquids (IL) were used as solvents for AB with the aim to provide an ionic medium for the decomposition reactions. The ionic liquids selected for this purpose are 1-Butyl-3-methylimidazolium Chloride (BmimCl), 1-Ethyl-3-methylimidazolium Ethyl sulfate (IoLiLyte 12IM), Trihexyltetradecylphosphonium bis(2,4,4-trimethylpentyl)phosphinate (TbmpMs) and 1-Ethyl-3-methylimidazolium acetate (Emim Acetate). We carry out temperature-programmed thermal decomposition of AB-IL mixtures where we simultaneously observed the mass-loss from the mixtures by thermal gravimetric analyzer (TGA), identified and quantified the impurity gases (ammonia, borazine and diborane) by infrared (IR) spectroscopy, and estimated the H_2 by mass spectroscopy (MS). The decomposition study reveals that AB in these ILs is able to yield nearly two equivalent H_2 below 110 °C. In contrary to the AB-Emim Acetate mixture where the most significant mass-loss is caused by ammonia, the thermal decompositions of AB in the other three ILs (IoLiLyte 12IM, BmimCl and TbmpMs) suggest that almost 90% of the mass-loss is caused by combination of the H_2 and the main three gas impurities. Less than 3% of AB molecules, in these three mixtures, decompose into ammonia and diborane whereas borazine comes from almost half of the AB molecules. The H_2 gas yields, in terms of equivalent of H_2, 2-2.4 in AB-IoLiLyte 12IM and AB-BmimCl, and approximately 1.9 in AB-TbmpMs are higher than 1.7 equivalent of H_2 produced from pure AB under the similar decomposition condition. Further improvements are important, especially, in the hydrogen yield and in reducing the impurities to near zero that may need to increase AB concentration in the suitable AB-IL mixtures while maintain the stability over a reasonable period of time as well the fluid nature of the mixture before and after the dehydrogenation. The present study may be an important initial step towards a realistic hydrogen fuel for the future automobile technology.

Materials Science and Technology Division
MST-6

Name	Edward Holby	LA-UR 12-20855
Groups:	MST-6 and MPA-11	
Mentors:	Chris Taylor and Piotr Zelenay	
Field of Study:	Materials Science	
Discipline:	Electrocheimstry/Catalysis	
Appointment:	Postdoc Research Associate	
Poster Title:	Non-Precious Metal Catalysts for Fuel Cells	

ABSTRACT

Low-temperature proton exchange membrane (PEM) fuel cells are a promising technology for clean energy generation for automotive use. One major hurdle for the widespread adoption of this technology is the use of rare and expensive platinum and platinum group precious metals as catalysts. The use of these materials dramatically increases the cost of PEM fuel cells and due to their limited supply, likely would not be able to meet the needs of a hydrogen fueled US automotive fleet. Consequently, suitable replacement of these catalysts is a field of very active research. These replacement catalysts are made of abundant materials such as iron, carbon, and nitrogen, hence their name, non-precious metal catalysts (NPMCs). These catalysts have traditionally suffered from poor catalytic activity but recent breakthroughs at Los Alamos National Lab have produced NPMCs rivaling the activity of precious metal catalysts. The molecular nature (composition, structure, and electronic state) of the active site where the relevant reactions take place is still unknown. Knowledge of this molecular nature would guide NPMC synthesis for increasing the number of active sites and potentially create a catalyst superior to even platinum at a considerably lower cost. Our research focuses on the identification of active sites through a combined experimental and theoretical approach. Experimentally, a variety of spectroscopic techniques are used to characterize NPMCs known to have high activity. Using quantum chemistry approaches, the theoretical studies propose potential active site candidates based on thermodynamic stability and then create spectra for these candidates that are directly comparable to experiments. This approach has produced a number of novel active site candidates not previously reported in literature that will be studied more in depth to determine their catalytic activity.



Name	Hieu Pham	LA-UR 12-21049
Groups:	MST-6 and T-1	
Mentors:	Chris Taylor and Neil Henson	
Field of Study:	Engineering	
Discipline:	Chemical Engineering	
Appointment:	Postdoc Research Associate	
Poster Title:	First-Principles Prediction of Thermodynamics and Kinetic Profiles of Carboxylic Acids in Organic Solvents	

ABSTRACT

Naphthenic acid is one of the major corrosive agents in the petrochemical industry. Naphthenic acid corrosion (NAC), as it is known, is of particular concern to oil transportation and refining facilities. Motivated by the recently increasing recovery of high acid crudes, there is a renewed interest in understanding the conditions controlling NAC due to the necessity of savings on production costs and improvement on the quality of crude oils. NAC is a high-temperature corrosion mechanism and is most active within the boiling range of the acids. No liquid water is required to initiate the corrosion.

In an initial effort to understand the NAC mechanism in petroleum medium, we have performed first-principles calculations of fundamental acid properties that emerge when the acids are dissolved in organic solvents (i.e. simulated crude oil). Acid dimerization and decarboxylation, which are believed to primarily occur at low and high temperatures, respectively, are important phenomena that determine the availability of free acid molecules and, therefore, may closely correlate to corrosion activity.

The stability of some model carboxylic acid systems was studied as a function of temperature and solvent selection. The Gibbs free energy of acid compounds in organic solvents at elevated temperatures was computed by adopting a technique that accounts for the thermal correction induced by entropy and enthalpy changes. Our calculations suggest that naphthenic acids have a high tendency to form cyclic dimers at low temperatures, but mainly exist in the monomer form at higher temperatures. In addition, the dielectric constant is a primary factor in determining the solvent effect.

A second theoretical study indicates that the decarboxylation process is thermodynamically very favorable but it is, however, totally controlled by kinetics. Our kinetics calculations, that simulate the thermal pyrolysis of acetic acid, excellently reproduce the experimental results.

Name	Matthew Rossi	LA-UR 12-20823
Group:	MST-6	
Mentor:	Chris Taylor	
Field of Study:	Chemistry	
Discipline:	Theory and Computation	
Appointment:	Postdoc Research Associate	
Poster Title:	Atomistic Modeling of the Role of Iodine in Stress Corrosion Cracking of Zirconium Alloys	

ABSTRACT

Existing fuel performance codes used by the nuclear industry today tend to favor empirical data, rather than deterministic physics-based models.[Lyon, W., Montgomery, R., Rashid, J., and S. Yagnik, PCI Analysis and Fuel Rod Failure Prediction using FALCON. Proceedings of Top Fuel, 2009: p. Paper 2125.] While these models are useful, the nature of semi-empirical values tends to incorrectly estimate effects that are fundamentally difficult to capture, such as chemical attack initiating at grain boundaries and subsequent susceptibility to corrosion. Part of the difficulty intrinsic to the existing semi-empirical values is due to the nature of experimental data, which may or may not include true reactor-condition based failures, such as those due to complex issues regarding not only chemical corrosion, but also irradiation damage, creep, and grid-to-rod-fretting. Additionally, sampling of the failed rods from reactor cores require a cooling period, during which much of the iodine may decay to other species, such as Xe and Cs, which may not still be present upon analysis of the rods. Iodine stress-corrosion cracking is one such failure model,[Atrens, A., Dannhäuser, G., and G. Bäro, Stress-corrosion-cracking of Zircaloy-4 cladding tubes. J. Nuc. Mater., 1984. 126: p. 91-102., Rudling, P., R. Adamson, Cox, B., Garzarolli, F., and A. Strasser, High burnup fuel issues. Nuc. Eng. & Tech., 2008. 40: p. 1-8.] for which empirical models have been developed, and yet, at the same time, physics based models are starting to emerge.[Legris, A. and C. Domain, Ab initio atomic-scale modeling of iodine effects on hcp zirconium. Phil. Mag., 2005. 85: p. 589-595., Lewis, B.J., Thompson, W.T., Kleczek, M.R., Shaheen, K., Juhas, M., and F.C. Iglesias, Modelling of iodine-induced stress corrosion cracking in CANDU fuel. J. Nuc. Mater., 2011. 408: p. 209-223.] In particular, the initiation stages of iodine-influenced stress corrosion cracking (ISCC) remain poorly understood; we seek to construct a physics-based model for the prediction of ISCC initiation, to be used in fuel performance modeling and simulation.

MST-8

Name	NFN Alankar	LA-UR 12-20870
Group:	MST-8	
Mentors:	Ricardo Lebensohn and Alfredo Caro	
Field of Study:	Materials Science	
Discipline:	Materials Engineering	
Appointment:	Postdoc Research Associate	
Poster Title:	A Multiscale Analysis of Dislocation Climb	

ABSTRACT

This work presents an analysis of dislocation-vacancy interaction in a pure Fe single crystal. By means of molecular dynamics simulations, we identify the unit processes that cause dislocation climb. The methodology suggests an improved determination of energy barriers that are used in kinetic-Monte Carlo simulations. The kinetic-Monte Carlo simulations show the effect of applied external stress on the vacancy concentration profiles around pure edge dislocation core. The flux of vacancy to dislocation core as a function of applied stress enables determination of stress exponent in the creep power law that is used in a continuum crystal plasticity model VPSC.

Name	Levente Balogh	LA-UR 12-20147
Group:	MST-8	
Mentors:	Donald Brown and Carlos Tome	
Field of Study:	Materials Science	
Discipline:	Neutron and X-ray Diffraction	
Appointment:	Postdoc Research Associate	
Poster Title:	Neutron Diffraction Studies of Dislocation Structure Evolution during Irradiation and Deformation of Zr-2.5Nb	

ABSTRACT

Zr-2.5Nb samples removed from a CANDU nuclear reactor are investigated using the high resolution Neutron Powder Diffractometer (NPDF) instrument at Los Alamos National Laboratory, to characterize the changes in dislocation structure induced by neutron irradiation. It is shown that Diffraction Line Profile Analysis (DLPA) is a valuable tool for the characterization of irradiated materials. The dislocation density is observed to increase from 6*10^14 to 24*10^14 m^-2 after 7 years of service, due to <a> Burgers vector type dislocations created by the neutron irradiation. DLPA also reveals a fundamental change in the arrangement of the dislocation structure induced by the irradiation compared to the cold worked, unirradiated state. The density of <a> Burgers vectors does not change during plastic deformation of the irradiated Zr-2.5Nb, while the <c+a> density increases sevenfold. This behavior indicates that part of the <a> Burgers vectors created by the irradiation participate in the plasticity of the material.

Name	Samrat Choudhury	LA-UR 12-20758
Group:	MST-8	
Mentors:	Blas Uberuaga and Christopher Stanek	
Field of Study:	Materials Science	
Discipline:	Computational Materials Science	
Appointment:	Postdoc Research Associate / Previous Director's Postdoc Fellow	
Poster Title:	Structure and Properties of the Y2O3/Fe Interface from First Principles Calculations	

ABSTRACT

To meet growing energy needs of the United States and the planet, more will be demanded of all energy technologies, including nuclear energy. Almost all of the advanced nuclear reactor concepts require operations under severe conditions of temperature, stress and radiation. To materials scientists, the primary challenge in realizing any of the advanced fission and future fusion energy systems is to design new high-performance structural materials for components -- such as the cladding and structural materials for fission reactors and first wall and blanket structural materials for fusion systems -- that can withstand such extreme operating conditions without compromising the structural integrity of the reactor over a long period of time. Nanostructured ferritic alloys (NFAs) are considered excellent candidate materials for such structural applications as they exhibit exceptionally high creep strength due to the presence of highly stable nanometer sized Y-Ti-O oxide precipitates within the primarily iron matrix. NFAs have also shown particular promise for their high radiation tolerance and ability to manage very high level of helium generated by transmutation reactions. It is believed that most of the radiation tolerance and He management properties in NFAs occurs at the metal/oxide interface. Thus an insight about the atomic structure of the metal/oxide interface is critical in understanding the origin of the enhanced properties of this material and ultimately designing new radiation resistant alloys.

Y2O3 has also been shown to form nanoprecipitates in iron and is a simpler surrogate for the Y-Ti-O precipitates. In this work, we present the behavior of the interface between the iron matrix and Y2O3 using density functional theory. In particular, the atomic structure of the interface will be presented. It was observed that, depending on the external partial pressure of oxygen, a critical number of defects -- iron-vacancies and/or interstitial oxygens -- are essential in stabilizing the metal/oxide interface. Importantly, the accommodation of these defects is very sensitive to the atomic structure of the interface, being enhanced at misfit dislocations at the interface. We discuss the implications of He storage at the interface in presence of such interfacial defects. Finally, we show the role of alloying elements, orientation relationship and interface misfit dislocations on the atomic and electronic structure of the metal/oxide interface, and segregation energies of the alloying elements. These results will form the basis of a phase-field model that will examine the nucleation and growth of Y2O3 precipitates in Fe. The insight gained in this research provides the fundamental science-based understanding needed to develop new NFAs tailored to meet challenges in fission and fusion applications, including safer operation of the current fleet of light water reactors.

Name	Saryu Fensin	LA-UR 11-06463
Group:	MST-8	
Mentors:	Ellen Cerreta, George Gray, and Steve Valone	
Field of Study:	Materials Science	
Discipline:	Shock Dynamics	
Appointment:	Postdoc Research Associate	
Poster Title:	The Role of Interfaces on Shock Induced Damage in Two-Phase Metals	

ABSTRACT

For ductile metals, the process of dynamic fracture during shock loading is thought to occur through nucleation of voids, void growth, and then coalescence that leads to material failure. Particularly for high purity metals, it has been observed by numerous investigators that voids appear to heterogeneously nucleate at grain boundaries. However, for materials of engineering significance, those with inclusions, second phase particles, or chemical banding; it is less clear what the role of grain boundaries versus other types of interfaces in the metal will be on nucleation of damage. To approach this problem two materials have been systematically investigated: (1) high purity copper, (2) copper with 1% lead. The role of lead at grain boundaries and its behavior during shock loading will be discussed in conjunction with the results from experiments and Molecular Dynamics simulations.

Name	Engang Fu	LA-UR 12-21342
Groups:	MST-8 and MPA-CINT	
Mentors:	Yongqiang Wang and Michael Nastasi	
Field of Study:	Materials Science	
Discipline:	Nuclear Materials	
Appointment:	Postdoc Research Associate	
Poster Title:	Radiation Response of Nano-Porous (np) Au Foams	

ABSTRACT

In this presentation, we report on experiments and computer simulations of the dose rate dependent irradiation response of nanoporous Au foams under Ne ion irradiations.

The co-deposited Au-Ag thin films on single crystal NaCl substrate by electron beam evaporation were first dealloyed to form Au foams by immersing them in dilute nitric acid. Then, the Au foams were irradiated by 400 keV Ne ions at different flux (dose rate) at room temperature. Rutherford backscattering spectrometry (RBS) was used to examine the composition and thickness of the Au-Ag thin films and transmission electron microscopy (TEM) was used to characterize the microstructure of the Au foams before and after ion irradiation. The results show significantly different behaviors of the defect accumulations by varying the flux. Stacking fault tetrahedra (SFTs) were observed in ion-irradiated np-Au foams at high radiation flux whereas no SFTs were found at very low radiation flux. The mechanisms to explain the observations are explored with computer simulations of the irradiation on the filaments.

Name	Tongsik Lee	LA-UR 12-21196
Groups:	MST-8 and MST-6	
Mentors:	Steve Valone and Chris Taylor	
Field of Study:	Physics	
Discipline:	Physics	
Appointment:	Postdoc Research Associate	
Poster Title:	Atomistic Modeling of Thermodynamic Equilibrium of Plutonium	

ABSTRACT

Among its six allotropes at ambient pressure, the fcc phase of plutonium, called delta-Pu, exhibits a wide range of anomalous behavior: extraordinarily high elastic anisotropy, largest atomic volume (despite the only close-packed structure among the allotropes), negative thermal expansion, strong thermal softening, and extreme sensitivity to dilute alloying. Thus far, there has been no first-principles method that correctly describes these unusual thermodynamic properties of plutonium. An elaborate modeling strategy at the atomic level can be an excellent alternative. We propose a novel atomistic scheme to model elemental plutonium and its alloys, in particular, to reproduce the anomalous characteristics of the delta-phase. Two modified embedded atom method potential are employed to represent the binding energies for competing electronic states in delta-Pu in order to embody the mechanism of the two-state model of Weiss. By the use of various techniques in Monte Carlo simulations, we are able to provide a unified perspective of seemingly diverse phenomenological aspects among thermal expansion, elasticity, and phase stability.

Name	Benjamin Morrow	LA-UR 12-20916
Group:	MST-8	
Mentors:	Ellen Cerreta and Carlos Tome	
Field of Study:	Materials Science	
Discipline:	Metallurgy	
Appointment:	Postdoc Research Associate	
Poster Title:	Variability in EBSD Statistics for Textured Zirconium	

ABSTRACT

Zirconium is an important structural material, and, as with other hexagonal close-packed (hcp) metals, the mechanical properties rely heavily on both the slip and twinning. Electron backscattered diffraction (EBSD), which can determine the relative orientations of each grain on a sample surface and return orientation maps and other statistics associated with active deformation mechanisms, has become a popular technique to characterize microstructure. Previous work in hcp metals has focused on identifying and quantifying twins found in deformed material to support development of physically based plasticity models. However, the data collection technique, including considerations arising from the unique crystal structure of hcp metals, has not been fully validated against potential sources of measurement artifacts or biases. Of particular interest are the potential differences arising from EBSD data as a function of viewing direction, especially for this highly textured metal. This work seeks to address these concerns by comparing results from three orthogonal directions in a deformed sample. Observed trends will be discussed, as well as ramifications for continued use of EBSD in this and similar materials.

Nuclear Nonproliferation Division
NEN-1

Name	Louise Evans	LA-UR 12-21064
Group:	NEN-1	
Mentor:	Martyn Swinhoe	
Field of Study:	Physics	
Discipline:	Neutron Non-Destructive Assay	
Appointment:	Postdoc Research Associate	
Poster Title:	The Euratom Fast Collar (EFC): A Safeguards Instrument Design to Address Future Fuel Measurement Challenges	

ABSTRACT

Neutron counting techniques are used for safeguards inspection measurements of fresh nuclear fuel assemblies in low-enriched uranium (LEU) fuel fabrication plants in Europe and the rest of the world. Measurements are performed for the independent verification of fissile ^{235}U mass in those assemblies. The instrument currently deployed for these measurements is the neutron collar, which wraps around a bulk fuel assembly. The neutron collar was originally designed by Los Alamos National Laboratory (LANL) and is now commercially available. In order to detect the presence of ^{235}U within the fuel assembly and quantify mass, the instrument uses an americium-lithium (AmLi) external neutron source to induce fission in the ^{235}U itself. Induced fission neutrons are then detected in ^{3}He tubes that surround the assembly on three sides and counted in data acquisition electronics.

Collar measurements have traditionally been performed using thermal neutron interrogation. However, thermal neutrons may be absorbed by integral fuel burnable poisons (e.g. Gd_3O_8). Thermal mode neutron collar measurements are thus sensitive to the presence of these poisons, which reduces the accuracy of the measurement. The alternate fast neutron interrogation, performed using a Cd liner within the instrument, reduces the sensitivity to the presence of burnable poisons but greatly increases the measurement time within current collar designs to a level that would not be acceptable for routine safeguards inspections. Therefore, as future fuel cycle needs drive fresh LEU fuel assemblies to become more complex, with different enrichment zones and widely varying poison rod distributions, the need for an improved measurement instrument is apparent. The requirements for a new instrument are such that it should be much less sensitive to poison rods and their distribution, and further be able to accumulate adequate statistical precision in an acceptable measurement time.

This poster presents the physics design of a new neutron collar detector that can verify ^{235}U mass in fresh LEU fuel assemblies with reduced poison sensitivity in a short (10 minutes) measurement time. Improving the instrument design mitigates the need to substantially increase the assay time. This instrument will be manufactured commercially and tested by the Euratom safeguards inspectorate.

Name	Danielle Hauck	LA-UR 12-20942
Group:	NEN-1	
Mentors:	Ernst Esch and Jonathan Thron	
Field of Study:	Engineering	
Discipline:	Arms Control Treaty Verification	
Appointment:	Postdoc Research Associate	
Poster Title:	The Role of Portal Monitors in Measurement Verification of Arms Control Treaties	

ABSTRACT

Measurement verification of arms control treaties is important for instilling confidence in compliance with treaty goals, and for demonstrating to non-nuclear weapon states, and all non-participating countries, that nuclear stockpiles are reduced. However, treaty verification is a complex problem, which involves interplay between technology and politics, and a conflicting relationship between the monitoring party which must verify the treaty obligations, and the host party, which must protect its own sensitive information. The aspects of authenticating a warhead declaration in an arms control scenario are described along with the ways in which different aspects of authentication interact with each other. The verification challenges that arise in a series of monitoring visits call for an integrated approach to monitoring regime authentication.

Portal Monitors are a key piece of technology, which represent a union between non-destructive analysis (NDA) and chain of custody (COC) in arms control verification. This linkage between NDA and COC is often neglected and the two areas are often erroneously treated as separate issues. In reality any system or protocol meant to address treaty verification must acknowledge the integration between NDA and COC. Design requirements and portal monitor implementations unique to an arms control scenario are described, including dual video surveillance-portal systems, triggered data recording and the potential need for information barriers on portal monitor data.

Name	Ryan Winkler	LA-UR 12-21313
Group:	NEN-1	
Mentor:	Michael Rabin	
Field of Study:	Physics	
Discipline:	Physics/Detector Development	
Appointment:	Postdoc Research Associate	
Poster Title:	Development of Microcalormeter Detectors for Nuclear Safegaurds and National Security Applications	

ABSTRACT

The development of ultra-high energy resolution cryogenic microcalorimeter detectors provides the opportunity for significant advances in the measurement accuracy and precision in a variety of nuclear safeguards and material accountability applications. These detectors have achieved energy resolutions for X- and gamma-ray spectroscopy as low as 22 eV at 100 keV, an order of magnitude improvement compared to current state-of-the-art high-purity Germanium (HPGe) detectors. The exceptional energy resolution of the microcalorimeter is derived from operation at low temperatures, typically near 100 mK. The foundation of these sensors is the transition-edge sensor (TES) thermally coupled to a bulk absorber with a superconducting quantum interference device (SQUID) readout. The improved resolution of microcalorimeter detectors is ideally suited for Plutonium isotopic measurements due to the spectral complexity of mixed-Actinide samples at energies below 200 keV and the intrinsic resolution limits of HPGe detectors. For X- and gamma-ray applications, a 256-pixel array of microcalorimeter detectors has been recently fabricated. Progress in the development of these novel detectors will be presented. Quantitative results of recent X- and gamma-ray spectroscopy and the direct comparison of the isotopic measurement precision for mixed-isotope Plutonium standards to HPGe measurements using newly developed software analysis tools will be presented.

NEN-2

Name	Sy Stange	LA-UR 12-01671
Group:	NEN-2	
Mentors:	Douglas Mayo and Paul Felsher	
Field of Study:	Engineering	
Discipline:	Nuclear Engineering	
Appointment:	Postdoc Research Associate	
Poster Title:	New Measurement Techniques for the Neutron POD	

ABSTRACT

Nuclear materials are commonly identified and characterized by analyzing the number and timing of the neutrons they emit. Using time-correlated neutron measurements and analysis techniques, the mass of the nuclear material, the neutron multiplication due to induced fissions, and its α-n ratio (an indicator of impurities) can be calculated. The Nuclear Nonproliferation Division has a long history of developing detector systems that can perform these measurements in support of domestic and international safeguards, emergency response, nondestructive analysis, and criticality safety. One of these systems is the Neutron POD. This detector consists of a total of 15 3He tubes in two offset rows. We have been exploring measurement techniques for this detector that make use of its geometry to provide information in addition to mass, multiplication, and the α-n ratio. These techniques include neutron spectrometry – determining the energy of incident neutrons – and using the Neutron POD to determine the direction of a neutron source. The results of directional and spectrometry measurements will be presented, as well as the methods developed to locate the direction of neutron sources and to identify the impurities present through incident neutron energies.

N-4

Name	Sara Kutchesfahani	LA-UR 12-00525
Group:	N-4	
Mentors:	Brian Boyer and James Doyle	
Field of Study:	Other	
Discipline:	Political Science	
Appointment:	Postdoc Research Associate	
Poster Title:	Next Generation Safeguards Initiative University Outreach: LANL Teaching a Political Science Course on Nuclear Safeguards and Security Policy at NM Tech	

ABSTRACT

One of the key pieces of the Next Generation Safeguards Initiative (NGSI) effort is to create and deliver university courses in safeguards. Political scientists from LANL created a course on "Nuclear Safeguards & Security Policy" to teach in the Spring 2012 semester at The New Mexico Institute of Mining and Technology. This course introduced students to the major themes and debates in the contemporary study of nuclear safeguards and security, from a historical perspective. Nuclear policy is a vast subject area and every week, the professors introduced students to one aspect of a range of topics covered throughout the 15-week course. Not only were the academic debates addressed, but so too were the contemporary policy debates. This way, students were exposed to both theory and policy. The course provided students with a broad overview of nuclear safeguards and security policy. The course required students to write two papers, lead one-side of the weekly debate topic in a seminar, and to actively participate in weekly seminars. Given that most of the students were technical and engineering students, already familiar with the technical aspects of safeguards, this course was designed to introduce the students to the political dimension of nuclear safeguards.

Physics Division
P-21

Name	Chaitanya Chandrana	LA-UR 12-20910
Group:	P-21	
Mentors:	Pulak Nath and Michelle Espy	
Field of Study:	Engineering	
Discipline:	Electrical Engineering	
Appointment:	Postdoc Research Associate	
Poster Title:	A Simple Magnet Assembly for Portable Nuclear Magnetic Resonance (NMR) Applications	

ABSTRACT

We present a simple, cost-effective permanent magnet assembly for portable Nuclear Magnetic Resonance (NMR) applications. Unlike traditional designs (e.g. Halbach) that use precisely aligned multiple magnets to generate uniform magnetic fields, this design utilizes only two components, a diametrically magnetized ring-shaped permanent magnet and a ferromagnetic co-axial shim. (We call them 'Shim-a-ring' magnets). The magnet and the ferromagnetic shim are self-aligned by magnetic attraction only. One of the major benefits of this shim-a-ring magnet is, it is highly scalable, and would not require high precision alignment to make pencil thin magnets for portable NMR applications. The model was designed and optimized using COMSOL 4.2a (COMSOL, Inc.). Prototypes were built using neodymium (NdFeB) magnets and low carbon steel, and tested. The devices produced sufficiently homogenous magnetic fields to measure localized proton spectra in a 0.54 T magnet. By adjusting the gap, ID and OD of the magnet and or shim, the field strength can be tuned upto an order of magnitude. Magnetic field measurements with hall probes agree with simulation results to within < 5%. NMR relaxometry was performed on water sample doped with CuSO4 using a custom probe. The probe is a 12 turn solenoid coil with a 0.32 mm diameter enameled magnet wire on a NMR tube (3.0 mm o.d. & 2.4 mm i.d.) and tuned to resonate at 22.89 MHz. The line width achieved, 550 parts per million is suitable for relaxometry applications. The initial results are encouraging and show promise for shim-a-ring magnets to become an integral part of different applications including lab on a chip.

Name	Todor Karaulanov	LA-UR 12-20945
Group:	P-21	
Mentors:	Igor Savukov and Michelle Espy	
Field of Study:	Physics	
Discipline:	Optics; Nuclear Magnetic Resonance	
Appointment:	Postdoc Research Associate	
Poster Title:	Optical Detection of NMR	

ABSTRACT

Nuclear magnetic resonance (NMR) revolutionized chemistry and biology with introduction of multi-dimensional spectroscopy that can deconvolute multiple interactions, for example, in proteins to obtain their structure. However, the quest for alternative methods for NMR detection has never stopped. Recently, by discovering the nuclear-spin optical rotation (NSOR) effect, we realized that optical spectroscopy can further enhance NMR spectroscopy by adding a new dimension in probing light-molecule interactions and interactions between excited atomic states and nuclear spins. NSOR is a result of the Faraday effect, in which a rotation of the plane of the polarization of a linearly polarized light occurs under the influence of the magnetic field produced by spin polarized nuclei. NSOR is enhanced by hyperfine interactions (which increase with the mass of the nucleus) thus making it a promising tool for study heavy nuclei.

In this presentation, we demonstrate our experimental results on optical detection of water NMR signal, where a significant improvement of sensitivity is achieved by using a blue laser, multi-pass cell geometry and sensitive polarimetry detection. The Verdet constant of water (the constant of proportionality between optical rotation and magnetic field strength) is measured using this technique.

P-23

Name	Nevzat Guler	LA-UR 12-21570
Groups:	P-23 and PADWP	
Mentors:	Frank Merill and Gary Grim	
Field of Study:	Physics	
Discipline:	Intertial Confinement Fusion	
Appointment:	Postdoc Research Associate	
Poster Title:	Nuclear Diagnostics at the Inertial Confinement Fusion Experiments at the National Ignition Facility	

ABSTRACT

Inertial Confinement Fusion experiments at the National Ignition Facility are designed to understand and test the basic principles of creating self-sustaining fusion reactions by laser driven compression of deuterium-tritium (DT) filled cryogenic plastic (CH) capsules. Experimental campaign is ongoing to understand the effects of various parameters on the characterization of ignition conditions. Nuclear diagnostics play an important role to measure some of these parameters and provide feedback to improve experimental design to accomplish ignition. The nuclear diagnostics are predominantly based on the observation of neutron, X-ray and Gamma-ray emissions during the nuclear burn. This poster presentation will primarily focus on the Neutron Imaging (NI) diagnostics, which provide vital information on the distribution of the central fusion reaction region and the surrounding DT fuel by observing neutron images in two different energy bands for primary (13-17 MeV) and downscattered (6-12 MeV) neutrons. From this, the final shape and size of the compressed capsule can be estimated and the symmetry of the compression can be inferred. In addition, the spatially averaged density of the nuclear fuel, which is another important parameter for optimizing the ignition conditions, can be calculated from these images during the peak neutron emission time.

This work was performed for the U.S. Department of Energy, National Nuclear Security Administration and by the National Ignition Campaign partners. Prepared by LANL under Contract DE-AC-52-06-NA25396. Prepared by LLNL under Contract DE-AC52-07NA27344.

Name	Patrick Younk	LA-UR 12-21548
Group:	P-23	
Mentors:	Brenda Dingus and John Pretz	
Field of Study:	Physics	
Discipline:	Astroparticle Physics	
Appointment:	Director's Postdoc Fellow	
Poster Title:	The Design and Construction of the HAWC TeV Gamma-ray Observatory	

ABSTRACT

Gamma-ray astronomy has the potential to shed light on many mysteries of the universe. Here I present some of the details of the design and construction of the HAWC TeV Gamma-ray Observatory, a new instrument under construction in Mexico. My particular contributions and involvement in the design and construction are highlighted.

P-25

Name	Sky Sjue	LA-UR 12-20953
Group:	P-25	
Mentors:	Mark Makela and Alexander Saunders	
Field of Study:	Physics	
Discipline:	Subatomic Physics	
Appointment:	Postdoc Research Associate	
Poster Title:	UCNB: Neutron Decay Correlation Measurements to Probe Physics Beyond the Standard Model	

ABSTRACT

The UCNB experiment is being developed with an ultimate goal to measure the energy dependence of the "neutrino asymmetry," B, from the decay of polarized ultracold neutrons (UCN) with 10^-4 precision for sensitivity to scalar and tensor interactions beyond the Standard Model. Large diameter, segmented Si detectors will be placed at opposing ends of a 1 Tesla decay volume to observe electrons and protons in coincidence. This will be an unprecedented implementation of segmented Si detectors for precision studies of neutron beta decay asymmetries and their energy dependence. These detectors have been used to measure a low energy proton beam at TUNL and to detect betas from UCN at Los Alamos. Progress toward full instrumentation of the detectors in the magnetic field with a bias voltage of 30 kV will be discussed. A preliminary experimental run to achieve a 10^-3 level measurement will be staged within the next year.

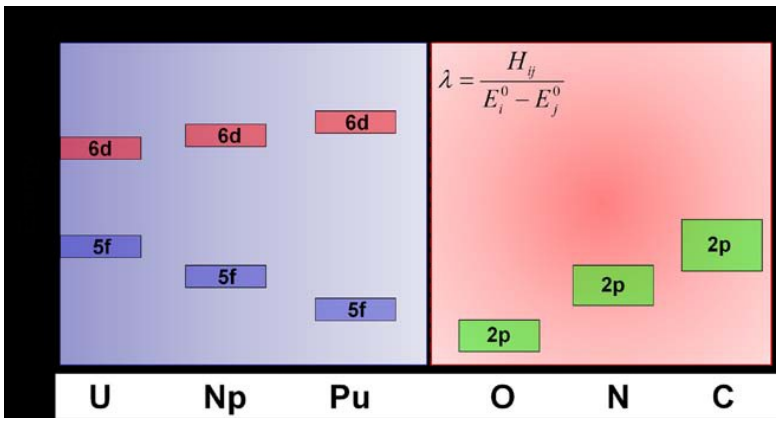
Theoretical Division
T-1

Name	Xiaodong Wen	LA-UR 12-20819
Group:	T-1	
Mentors:	Richard Martin and Sven Rudin	
Field of Study:	Chemistry	
Discipline:	Catalysis	
Appointment:	Postdoc Research Associate	
Poster Title:	Screened Hybrid Density Functional Prediction for Actinide Materials	

ABSTRACT

The actinide oxides, nitrides, and carbides are of both fundamental and applied interest. A number of basic properties associated with their electronic structure are still not known; this includes magnetic ordering, optical gaps, and resistivity and so on. In the work, we systemically investigate structural and electronic properties of actinide materials across from oxides to nitrides to carbides via performing Screened Hybrid Density Functional (HSE) approach which have met with some success in the Mott insulators.

Our computed results show that the hybrid HSE functional gives a better description of the electronic (magnetic states, density of states, band gap and optical properties, etc.) and structural properties (lattice constant, bond length, etc.) for actinide dioxides, strongly correlated insulator series when compared with available experimental data from our collaboration groups at LANL. However, there are still some problems on predicting the electronic properties of actinide nitrides and carbides which mainly fall in strongly correlated metals, indicating that screened hybrid DFT is missing key physics for the remaining piece of the puzzle, the correlated metallic regime. In addition, to compare with the results by HSE, the structures, electronic and magnetic properties of these actinide compounds are also investigated by performing PBE and PBE+U approximation. Roughly speaking, PBE gives a wrong prediction on the ground states of these materials and electronic properties of Mott insulators, however, it offers a good description on electronic properties for the correlated metallic systems. In a certain way, the prediction on electronic structure from PBE+U is similar to those by HSE, while the computed lattice constants by PBE+U are far away from these values. HSE values are in good agreement with the experimental data.



Scheme 1. Illustrated energy levels for U, Np, Pu and O, N, C.

Name	Andriy Zhugayevych	LA-UR 12-20930
Group:	T-1	
Mentors:	Enrique Batista and Sergei Tretiak	
Field of Study:	Materials Science	
Discipline:	Organic Solar Cells	
Appointment:	Postdoc Research Associate	
Poster Title:	First-Principles Study of Energy and Charge Transport in Molecular Donors for Organic Solar Cells	

ABSTRACT

Solar radiation is one of the easiest sources of energy to access but is one of the most expensive sources to convert to electricity. Organic solar cells hold promise as low-cost photovoltaic devices. To achieve this goal the power conversion efficiency should be increased to about 15% which is theoretically possible for currently used materials.

A low-cost implementation of organic photovoltaic devices is based on bulk-heterojunction of pi-conjugated molecular donor and fullerene-based acceptor: the solar radiation is absorbed by the first component resulting in the creation of an exciton migrating to the interface where the exciton is split into the hole and electron transported to the electrodes by the donor and acceptor respectively. The complex multiscale morphology of this device limits the ability of experimental approaches to pinpoint the power conversion losses and thus to avoid the blind search of highly efficient devices. In this situation a theoretical study becomes an essential complementary tool of investigation.

We perform first-principles study of light absorption, exciton and charge carrier transport in polycrystalline small-molecule based donors. Our results show that there are no power conversion losses on a single-crystallite scale. Thus the main efforts should be put in improving the mesoscale morphology of the active layer.

T-2

Name	Jarrett Johnson	LA-UR 12 -21186
Groups:	T-2 and CCS-2	
Mentors:	Hui Li and Christopher Fryer	
Field of Study:	Astronomy	
Discipline:	Theoretical astrophysics and cosmology	
Appointment:	Director's Postdoc Fellow	
Poster Title:	The Supermassive Stellar Seeds of Black Holes	

ABSTRACT

The collapse of the primordial gas into supermassive stars with masses ~ 10^5 that of the sun is a popular scenario for the origin of supermassive black holes that are inferred to power quasars within the first billion years after the big bang. Here we address two key questions with regard to the formation of supermassive stars and the black holes to which they collapse. Firstly, how large can such stars grow? And, secondly, how often do they form in the early universe? To address the first, we have modeled analytically the impact of the radiation emitted by the star on the accretion flow which feeds its growth, and we find that for the high accretion rates that are expected, stars can easily grow to at least ~10^5 solar masses. To address the second, we have carried out large-scale cosmological simulations in which we track in detail the chemical, mechanical, and radiative feedback from stars in the early universe, which allows us to pinpoint the sites at which supermassive star formation is possible. We find that the conditions for supermassive star formation are satisfied much more often than previously expected. Overall, our work strongly supports supermassive star formation as a valid, and perhaps widespread, mechanism of supermassive black hole formation.

Name	Yi-Hsin Liu	LA-UR 12-20806
Groups:	T-2 and XCP-6	
Mentors:	Hui Li and William Daughton	
Field of Study:	Physics	
Discipline:	Astrophysical and Space Plasma Physics	
Appointment:	Postdoc Research Associate	
Poster Title:	The Tearing Instability and Reconnection at Force-Free Harris Geometry in 3D PIC Simulations	

ABSTRACT

While most studies of magnetic reconnection have focused on Harris-type equilibrium, which is relevant to the Earth's magnetosphere, there has been growing interest in force-free current sheets. This type of initial condition is thought to be more relevant when the energy density in the magnetic field greatly exceeds the thermal energy of the plasma. This is clearly the case in hot solar corona of our Sun, and it is also thought to be true within the relativistic jets emerging from AGN. In force-free layers, the current flows parallel to the strong local magnetic field while the density is uniform. This is very different from the Harris sheet initial condition. However, there has been limited work on kinetic studies of magnetic reconnection in such force-free configurations. One important first step is to understand the 3D evolution of tearing modes (or magnetic flux ropes in 3D simulations). It has been hypothesized that a spectrum of these interacting islands may play a crucial role in accelerating energetic particles, either though coalescence or through Fermi acceleration inside contracting islands. Thus, it is very important to understand how many magnetic flux ropes are produced within a given large-scale current sheet that goes unstable to reconnection. Accordingly, we have completed a detailed linear stability analysis of the tearing mode for the force-free configuration and verified the mode properties using 2D full particle simulations and 3D Fourier spectrum. This theory shows that the tearing modes are unstable over a wide range of oblique angles. Recently, the interaction of oblique modes in a Harris current sheet leads to turbulent magnetic reconnection is demonstrated [1]. In the force-free configuration, our linear theory predicts much more power in oblique modes than in the Harris equilibrium. These results suggest that force-free current sheets may be even more susceptible to the generation of turbulent flux ropes during magnetic reconnection in large 3D systems. [1] Daughton et al. Role of electron physics in the development of turbulent magnetic reconnection in collisionless plasmas. Nature Physics, 7, 539, 2011.

T-3

Name	Jonathan Pietarila Graham	LA-UR 12-20740
Group:	T-3	
Mentor:	Todd Ringler	
Field of Study:	Physics	
Discipline:	Computational (Magneto) Fluid Dynamics	
Appointment:	Postdoc Research Associate	
Poster Title:	Not Much Helicity is needed to Drive Large Scale Dynamos	

ABSTRACT

Understanding the in situ amplification of large scale magnetic fields in turbulent astrophysical rotators has been a core subject of dynamo theory. When turbulent velocities are helical, large scale dynamos that substantially amplify fields on scales that exceed the turbulent forcing scale arise, but the minimum sufficient fractional kinetic helicity f_h,C has not been previously well quantified. Using direct numerical simulations for a simple helical dynamo, we show that f_h,C decreases as the ratio of forcing to large scale wave numbers k_F/k_min increases. From the condition that a large scale helical dynamo must overcome the backreaction from any non-helical field on the large scales, we develop a theory that can explain the simulations. For k_F/k_min>8 we find f_h,C< 3%, implying that very small helicity fractions strongly influence magnetic spectra for even moderate scale separation.

T-4

Name	Tanmoy Das	LA-UR 11-07009
Group:	T-4	
Mentor:	Matthias Graf	
Field of Study:	Physics	
Discipline:	Theoretical Condensed Matter and Material Science	
Appointment:	Postdoc Research Associate	
Poster Title:	Spin-Orbit Coupling Density Wave: A New Paradigm of Quantum Mechanical Phase of Matter	

ABSTRACT

When a correlated system is cooled from high-temperatures, its electronic degrees of freedom melt into new kinds of phase that are often characterized by broken symmetries. The emergent phases are usually described by standard quantum numbers in the spin, orbital, momentum channels. On the other hand, there exists a large class of materials in which the electronic spin is locked to its orbital or momentum via various types of spin-orbit coupling. In such cases, the electronic ground state is defined by more exotic quantum numbers such as total angular momentum, pseudospin, helical index. When Coulomb interaction is turned on in such systems, we propose that novel emergent phases may appear which break symmetries in different ways. A most favorable state is density wave order which appears when the translational periodicity of the crystal is spontaneously broken. We will be calling such state in general as spin-orbit coupling density wave. We apply our idea to two different systems having different types of spin-orbit coupling: to the long-standing puzzle of the 'hidden-order' state in actinide materials having j-j spin-orbit coupling (j is the total angular momentum) and to the two-dimensional electron gap where Rashba-type spin-orbit coupling appears. Taken together, we put forward an interaction induced spin-orbit coupling state which is highly desired and relevant for studying emergent new physical properties as well as for spin-based transport and quantum information application.

Name	Jason Haraldsen	LA-UR 12-00591
Group:	T-4	
Mentor:	Alexander Balatsky	
Field of Study:	Physics	
Discipline:	Condensed Matter Physics	
Appointment:	Postdoc Research Associate	
Poster Title:	Evidence for a Hidden-Order Pseudogap in URu_2Si_2	

ABSTRACT

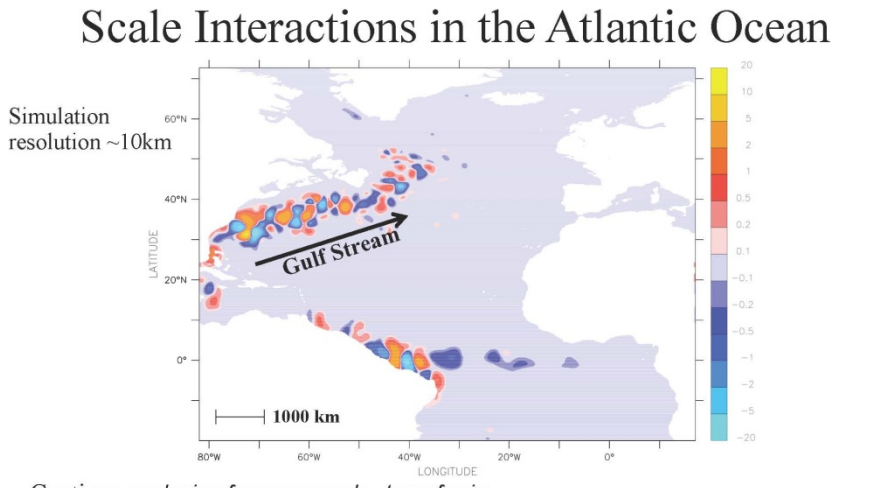
Through an analysis and modeling of data from various experimental techniques, we present clear evidence for the presence of a hidden order pseudogap in URu_2Si_2 that exists in the temperature range between 17.5 K and 25 K. By considering fluctuations of the hidden order energy gap at the transition point, we evaluate the effects that gap fluctuations would produce on observables like tunneling conductance, neutron scattering and nuclear resonance. These simulations are then related to the known experimental findings in literature. We show that the transition into hidden order phase is likely second order and is preceded by the onset of non-coherent hidden order fluctuations produced by competing orders.

T-5

Name	Hussein Aluie	LA-UR 12-20603
Group:	T-5	
Mentors:	Susan Kurien	
Field of Study:	Engineering	
Discipline:	Fluid Mechanics and Turbulence	
Appointment:	Postdoc Research Associate	
Poster Title:	Compressible, Magnetohydrodynamic, and Geophysical Turbulence: Analyzing Nonlinear Scale Interactions	

ABSTRACT

We utilize a coarse-graining framework, rooted in a commonly used technique in the subjects of PDEs and large eddy simulation modeling, to analyze nonlinear scale interactions in flow fields. The approach is powerful and very general, allows for probing the dynamics simultaneously in scale and in space, and is not restricted by the usual assumptions of homogeneity or isotropy. The method allows for quantifying the coupling that exists between different scales through exact mathematical analysis and numerical simulations, and may be used to extract certain scale-invariant universal features in the dynamics. We apply these multiscale analysis tools to study (1) compressible turbulence, (2) magnetohydrodynamic turbulence, and (3) geophysical flows.



Caption: *analysis of energy scale- transfer in the North Atlantic from a high-resolution POP simulation. The flow is very inhomogeneous with prominent nonlinear transfer in the Gulf Stream. Red (blue) is energy transferred from scales larger (smaller) than ~200 km to scales smaller (larger) than ~200 km.*

Collaborators:
R. Ecke, M. Hecht, M. Maltrud, B. Wingate (LANL)
K. Bryan, G. Vallis (Princeton)

Name	Ethan Coon and Mark Porter	LA-UR 11-11721
Groups:	T-5 and EES-14	
Mentor:	David Moulton	
Field of Study:	Mathematics and Computer Science	
Discipline:	Computational Geosciences	
Appointment:	Postdoc Research Associate	
Poster Title:	Taxila LBM: A Lattice-Bolzmann Simulator for Single and Multi-Phase Flow in Complex Porous Media	

ABSTRACT

It has been recognized that many of the assumptions underlying conventional continuum models for flow and transport in porous media are not always met for engineering problems of practical interest. Thus, modeling efforts that couple the pore-scale to the continuum (Darcy) scale through upscaling or hybrid modeling have recently gained interest. Such problems are inherently computationally expensive, as resolving micro-scale features within a continuum-scale domain, even in localized regions, requires significant resources. In this work, we introduce the LANL, open source simulator Taxila LBM -- a parallel, lattice Boltzmann simulator for single-phase, multi-phase, and multi-component flow through complex porous media. First, we discuss the implementation of the LB method and some of the more advanced features, including multiple relaxation times, higher order isotropy in inter-fluid forces, mixed wettability, and various equations of state. Next we demonstrate the capabilities of Taxila LBM with some examples.

In addition, Taxila LBM has been coupled to PFLOTRAN, a continuum scale multi-phase flow and reactive transport simulator, where the reactive-transport equations in PFLOTRAN have been modified to work at the pore-scale. In this coupling, flow is simulated using Taxila LBM, while multi-mineralic and many-species reactions are simulated using PFLOTRAN. We present examples of reacting flows which are not well-mixed at the pore-scale, and discuss implications for common assumptions at the continuum scale.

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Groups:	T-5 and ISR-3	
Mentors:	Rick Chartrand and Steven Brumby	
Field of Study:	Mathematics and Computer Science	
Discipline:	Machine Learning; Neural Computation; Computer Vision	
Appointment:	Postdoc Research Associate	
Poster Title:	Unsupervised Learning of Visual Representation for Object Identification and Vision-Based Navigation	

ABSTRACT

Learning good feature representation (rather than pixels) is a fundamental goal in computer vision. Many computer vision methods rely on the availability of labeled data to produce feature representations from inputs. While labeled data is very expensive to get and sometimes too scarce to fit a model in real-world application (e.g., high-dimensional video analysis), unlabeled data can often be obtained in large scale at very low cost. In this talk, I will describe a class of unsupervised learning methods to generate good internal representation from unlabeled data. The approach is based on a generalization of generative models with sparse constraints, which emphasizes feedback processes as generators of local image predictions in hierarchical architectures. The Bayesian framework is utilized to address visual inference in the hierarchical structure, where each cortical area is an expert for inferring certain aspects of the visual scene. The learned sparse internal representations show favorable performance in vision tasks of generic object identification and vision-based autonomous navigation. The general principle of unsupervised sparse learning can also be applied to other domains than vision, such as biomimetic odor discrimination, text document retrieval and classification, etc.

Weapons Experiments Division
WX-9

Name	Patrick Bowden	LA-UR 12-20956
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Mentor:	Dana Dattelbaum	
Field of Study:	Chemistry	
Discipline:	Static High Pressure	
Appointment:	Postdoc Research Associate	
Poster Title:	Terahertz Spectroscopy of Explosives under Static High Pressure	

ABSTRACT

THz-frequency (0.1-10 THz or 3.3-334 cm^{-1}) radiation, and the resulting spectral signatures in the same frequency regime, has been proposed for the detection of explosives, due to its specificity, and ability to penetrate non-metallic materials. To investigate the sensitivity of THz modes to environmental factors such as temperature, pressure, and mechanical or electrical perturbations, we have performed synchrotron-based THz transmission measurements of 7 explosives (TNT, RDX, HMX, PETN, R-salt, AN, and TNB) at high pressure in optically-transparent diamond anvil cells (DACs). Using type-IIa diamonds mounted in DACs, THz-to-far-infrared transmission spectroscopy was performed on explosive samples ~200 microns thick x 500 microns in diameter. The NSLS VUV beam line at Brookhaven National Laboratory was employed to supply a sufficient light source for transmission experiments in the THz and far-IR (60-600 cm^{-1}) region. The results show a high degree of sensitivity of the modes to applied pressure. In addition to peak shifts of up to 20 cm^{-1}/GPa (gigapascal), significant peak broadening and eventual disappearance was observed for most of the explosives tested – a pressure-driven THz transparency. New vibrational spectroscopy data were also obtained for several of the explosives using both Raman spectroscopy and mid-IR transmission measurements (600-4000 cm^{-1}). These data are important for identifying structural phase transitions at high pressure, and for informing thermodynamic equation of state models for explosives.

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Discipline:	High Pressure-Temperature Materials Chemistry	
Appointment:	Postdoc Research Associate	
Poster Title:	Mapping the P-T Stability of Energetic Materials & their Building Blocks: Insights into Shock Sensitivity from Static Compression	

ABSTRACT

A fundamental understanding of shock-induced molecular-level processes during the evolution from shock initiation to steady-state detonation of energetic molecular crystals is still lacking. There is a complex interplay of various factors including macroscopic inelastic deformation & crystal defects and molecular-level reactivity of chemical bonds enhanced due to high compressibility and rapid rise in temperature. A key experimental obstacle to investigate these phenomena directly under shock compression is the fast timescale of reactions that necessitates challenging diagnostics to fully quantify the mechanisms involved. Static compression (using Diamond Anvil Cell: DAC) provides a complementary route to gain insights into shock-induced phenomena by allowing us to investigate the equilibrium pressure-temperature (*P-T*) phase space, establish structural evolution, and occurrence of reactive metastable intermediates. Due to slow timescale of static compression studies, we can use a suite of experimental structural and spectroscopic tools to carefully probe molecular-level interactions in energetic materials. In addition to generating critical *P-V-T* Equation of State (EOS) data, the high *P-T* stability of various polymorphs of these energetic compounds can aid in the interpretation of their shock sensitivity and response. Further insights can be gained by investigating high *P-T* behavior of aromatics (nitrobenzene (mono-, di-), toluene, aniline, and others) with C-NO2, C-NH2, and CCH3 bonds that also constitute advanced energetic materials such as Triaminotrinitrobenzene [TATB: C6H6N6O6], Diaminoazoxyfurazan [DAAF: C4H4N8O3], and others. The aromatics can be construed as building blocks of these insensitive high explosives (IHEs).

In this study, we will present results from our ongoing studies to map the phase diagrams and obtain *P-V-T* Equation of State (EOS) of IHEs including TATB and DAAF as well as ammonium nitrate [AN: NH4NO3], a non-ideal explosive. The high *P-T* phase boundaries of AN were established by characterizing phase transitions to the high temperature polymorphs during multiple *P-T* measurements using synchrotron x-ray diffraction (XRD) and Raman spectroscopy measurements. This is only the third known phase diagram study and the first revision in over five decades for an extremely important non-ideal explosive that is widely used in industrial and military formulations as well as improvised explosive devices (IEDs). The stability of ambient pressure orthorhombic (*Pmmn*) AN-IV phase over a large *P-T* phase space, steep phase boundaries, and anomalous thermal expansion at high pressures are used to explain the lack of shock initiation up to 22 GPa. We have also revised the EOS for DAAF and TATB up to 20 GPa and 45 GPa, respectively. Hydrogen bonding is observed to play a key role in the high pressure stability of these compounds and we will highlight some key insights obtained from our studies on nitrobenzene and aniline building block molecules.

Name	David Fredenburg	LA-UR 12-20968
Group:	WX-9	
Mentor:	Darcie Dennis-Koller and Paulo Rigg	
Field of Study:	Physics	
Discipline:	Shock Compression	
Appointment:	Agnew National Security Postdoc Fellow	
Poster Title:	Consolidation Response of Brittle Particulate Materials at Low- and High-Strain-Rates	

ABSTRACT

The shock consolidation response of brittle particulate materials is a complex process that is influenced by many factors, inclusive of the initial packing density and the size and shape of particles and voids. In this work, the shock consolidation and high-pressure equation of state response of several different morphology CeO2 powders is investigated. The measured response under dynamic and quasi-static loads are correlated with initial microstructural features. Examination of compacted microstructures following quasi-static loading reveals varying levels of deformation and fracture of the particles, with the largest particles exhibiting the highest levels of both. Characteistics of the continuous compaction curves at low, intermediate, and high (< 1 GPa) pressures are also analyzed with respect to evolving microstructural features. Parallel plate impact experiments are performed on each of the morphologies, and the compaction responses are found to exhibit a broad distribution in densificaiton paths. At pressures below those required to reach full density, significant differences are observed between the quasi-static and dynamic loading paths. A transition in compliance between the particles is observed as loading rates are increased, and suggest that the compaction response shifts from shape controlled to size controlled as loading transitions from quasi-static to dynamic.

Name	John Yeager	LA-UR 12-20349
Group:	WX-9	
Mentor:	Daniel Hooks	
Field of Study:	Materials Science	
Discipline:	Structure-Property Relationships in Composites	
Appointment:	Agnew National Security Postdoc Fellow	
Poster Title:	Mesoscale Characterization of Plastic-Bonded Explosives across Time and Length Scales	

ABSTRACT

Understanding and predicting detonation and failure mechanisms in plastic-bonded explosives (PBX) is a key area of research for the DOE and DoD. Defects within explosive crystals, at the crystal-binder interface, in the partially-dissolved crystal-binder region ("dirty binder"), or within the binder itself may all contribute to "hot spot" formation and initiate deflagration or detonation in off-normal conditions. A mesoscale interpretation of the microstructure and its contribution to PBX properties is necessary to inform PBX damage and mechanical behavior models, to understand and predict failure of current explosives, and to design better explosives for future use. This research investigates the microstructural contributions to quasi-static and dynamic PBX behavior, with focus on the crystal-binder interface. Several PBX formulations are studied to illustrate the effectiveness of the characterization methodology. Engineered PBX 9501 composites were studied with neutron reflectometry, showing that the nano-structure at the crystal-binder interface was altered when a plasticizing agent was included in the formulation. The plasticized interface resulted in worse adhesion between the binder and the crystal as quantified with quasi-static nanoindentation and atomic force microscopy. Similar results were found for explosive formulations PBXN-9 and Composition A-3, along with several pharmaceutical composites, showing the applicability of these techniques to a variety of materials. Dynamic behavior of inert composites was studied at high resolution (2 um pixel size) with time-resolved synchrotron X-ray phase contrast imaging (PCI). PCI was first used for static microstructural characterization, showing that defects such as bubbles, voids, cracks, surface defects, and binder delamination were all observable even with microsecond exposures. Dynamic behavior was studied by combining a light gas gun with ultrafast PCI (60 picoseconds) using the IMPact system for Ultrafast Synchrotron Experiments (IMPULSE) at the Advanced Photon Source. Shock events such as dynamic cracking, massive plastic deformation, spallation, and impact were clearly observed even at these ultrafast time scales. These characterization techniques show the ability to establish relationships between formulation processing, mesoscale structure, and mechanical properties from static to ultrafast regimes.

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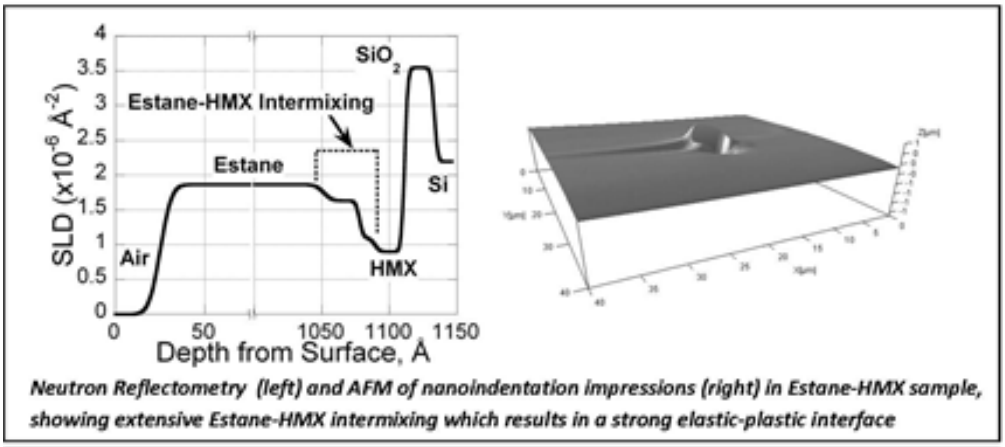
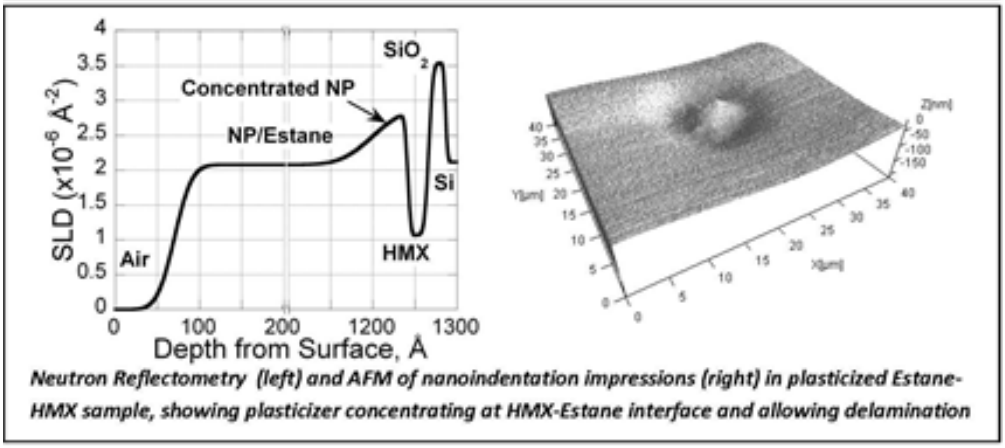
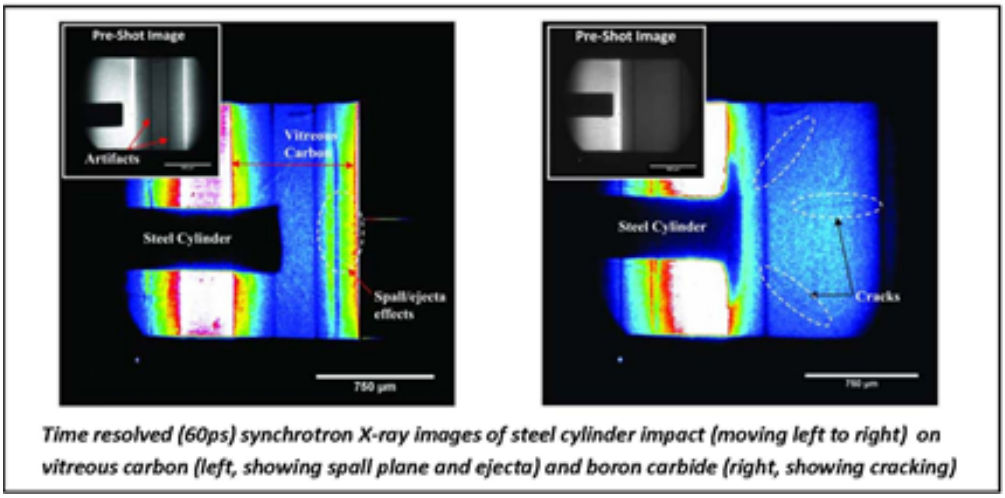
Poster Title:	Mesoscale Characterization of Plastic-Bonded Explosives across Time and Length Scales	



Neutron Reflectometry (left) and AFM of nanoindentation impressions (right) in Estane-HMX sample, showing extensive Estane-HMX intermixing which results in a strong elastic-plastic interface



Neutron Reflectometry (left) and AFM of nanoindentation impressions (right) in plasticized Estane-HMX sample, showing plasticizer concentrating at HMX-Estane interface and allowing delamination



Time resolved (60ps) synchrotron X-ray images of steel cylinder impact (moving left to right) on vitreous carbon (left, showing spall plane and ejecta) and boron carbide (right, showing cracking)

X-Computational Physics Division
XCP-4

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Field of Study:	Mathematics and Computer Science	
Discipline:	Fluid Dynamics	
Appointment:	Postdoc Research Associate	
Poster Title:	Turbulence Modeling in the FLAG Hydrocode	

ABSTRACT

Fluid turbulence is a ubiquitous phenomenon in nature, and the mixing of multiple materials is important in situations ranging from stirring cream into coffee to inertially confined fusion (ICF). Many researchers have spent a great deal of effort developing models of the turbulent mixing process. Los Alamos National Laboratory has developed and validated a family of turbulence models known as BHR[1] to describe this process. Thus far this work has focused on the implementation of BHR in the "Eulerian" framework. That is, the fluid motion is computed with respect to a grid that is fixed in space.

In addition to this Eulerian framework, there are research codes at the Laboratory that operate in a "Lagrangian" framework, where the grid moves with the fluid. Efforts are underway to establish mix-models that are common across various codes. For that goal, it is important that the BHR model be implemented and validated in a Lagrangian hydrocode.

FLAG is a fully-unstructured, compressible, hydrodynamics code that operates in an Arbitrary Lagrangian-Eulerian (ALE) framework, with a Lagrange step followed by mesh relaxation and remapping as needed. The poster gives the basics of FLAG and the BHR implementation, and describes validation studies performed thus far. Specifically, the BHR model in FLAG is compared to solutions from the Eulerian code xRAGE for simple mixing problems, as well as with experiments and high resolution simulations for mixing with a tilted interface.

These simulations are based on the tilted rocket-rig experiments[2] designed to study mixing of fluids by the Rayleigh-Taylor instability. In the traditional Rayleigh-Taylor instability, a heavy fluid is placed above a light fluid under the influence of gravity. This situation is unstable, and interface between the fluids quickly begins to mix. An additional complication is introduced in the tilted-rig experiment. Here, a tank containing two fluids of different densities is accelerated downward (simulating strong gravity) with the rig inclined by a few degrees off vertical. The result of this is that not only do the two fluids mix, but the interface itself begins to turn over. Thus the experiment can be compared to the numerical simulations and we can analyze the ability of models to correctly capture the 2D flow features.

References:
[1] Stalsberg-Zarling, K. and Fore, R., LA-UR 11-04773, LANL, 2011
[2] Smeeton, V.S. and Youngs, D.L., AWE Report No. 0 35/87, 1987

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Mentor:	Fernando Grinstein	
Field of Study:	Physics	
Discipline:	Fluid Dynamics	
Appointment:	Metropolis Postdoc Fellow	
Poster Title:	Reynolds-Averaged Navier-Stokes Model Initialization and Validation in Shock-Driven Turbulent Mixing	

ABSTRACT

We report progress in developing a working framework for testing and design of unsteady engineering model initialization and closures for fluid simulations of shock-driven turbulent material mixing based on comparing moments extracted from ensemble-averaged three-dimensional large-eddy simulation (LES) data and those predicted directly by a two-dimensional, variable-density, compressible, Reynolds-Averaged Navier-Stokes (RANS) model. The prototypical shock-tube considered is the inverse chevron shock-tube configuration for which laboratory and LES studies have been previously reported. Simulation strategies use implicit LES based on LANL's RAGE hydrodynamics code and a multi-equation unsteady RANS (BHR) model. New LES results are validated through comparison with previous simulations and available experimental data; sensitivity to initial material interface conditions, grid resolution, and artificial diffusion options in RAGE are addressed. The RANS approaches tested are capable of capturing various integrated quantities of the flow when compared to the ILES data; sensitivities to RANS initialization details as well as model and closure specifics are examined in this context.